

Techno-economic and environmental evaluation of lignocellulosic biochemical refineries: need for a modular platform for integrated assessment (MPIA)

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Ethanol production from lignocellulosic residues has potential to significantly improve sustainability of biofuels for transport by avoiding land-use competition with food crops and reducing impacts related to agricultural inputs. However, high production costs remain bottleneck for large-scale development of this pathway. A huge potential exists in upgrading energy producing pathways into biorefineries in order to improve its economic performance and long-term sustainability. A promising general model for a lignocellulosic biochemical refineries (LCBR) is based on sugar-lignin platform, in which 5-carbon (C5) and 6-carbon (C6) sugars, resulting from lignocellulosic matrix fractionation, are converted into fuels and building block chemicals by biotechnological or chemical pathways. In this context, comprehensive, flexible and dynamic modelling approaches are needed to solve a problem with multiple optimization criteria (economic and environmental), high levels of uncertainty and dynamic behaviour. Process simulators and comprehensive databases of production processes can help to determine rigorous and thermodynamically consistent material and energy balances permitting robust scale-up and reducing uncertainty in economical and environmental impact evaluation in a dynamic context. This paper discusses the need for developing a modular platform for process synthesis aiming at selection of technically, economically and environmentally sound pathways for lignocellulosic biorefineries.

Keywords: Biofuels, Biorefineries, Optimisation, Process design

Introduction

Lignocellulosic biomass¹ (LB) resulting from agro-industrial residues from corn, barley, oat, rice, wheat, sorghum and sugarcane could produce up to 442 Gt of bioethanol per year. A promising general model for a lignocellulosic biorefinery is based on sugar-lignin platform, in which 5-carbon (C5) and 6-carbon (C6) sugars, resulting from lignocellulosic matrix fractionation into its main components (hemicellulose, cellulose and lignin) are converted into fuels and building block chemicals by biotechnological or chemical pathways (Table 1). Cellulose is recalcitrant to biodegradation and needs to be hydrolysed in an initial pretreatment step into its constituent cellobiose units and into simpler D. glucose units in order to be liable to biochemical conversion. Hemicellulose components are rapidly solubilised and include polysaccharides such as xylan - composed of xylose units, a C5 sugar- and mannan - composed of mannose units, a C6 sugar-, intertwined

with acetate groups that can be easily solubilised into acetic acid during pretreatment step. Ethanol production from LB can be considered as backbone of lignocellulosic biochemical refineries (LCBR) (Fig. 1).

For first generation biofuels, feedstock represents a high share of production costs (70%), which is not the case for second generation biofuels, in which the share decreases and becomes less than 40%^{2,3}. High production costs and technological uncertainties remain bottleneck for large-scale development of this pathway that will increasingly depend on environmental and social concerns as well as on economic factors^{2,4}. Crucial steps are pretreatment and saccharification coupling with fermentation stage^{2,5}. An ideal pretreatment step⁶ should yield a hydrolysate with undegraded pentoses, reduced production of fermentation inhibitors and exhibiting a good suitability to work at high solid/liquid ratio. National Renewable Energy Laboratory (NREL) models^{7,8}, developed in close cooperation with highly experienced enzyme producers (Novozymes Biotech), include dilute acid as pretreatment, consider hardwood and agricultural residues as feedstock, show different levels of process

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Table 1—Few technological non-exclusive options for different process stages of lignocellulosic biochemical processing into ethanol

Process stage	Technological variant
Pretreatment	AFE (Ammonia fiber explosion); Concentrated acid hydrolysis; Dilute acid hydrolysis; Alkaline hydrolysis; Milling; Steam explosion; Autohydrolysis
Cellulose hydrolysis and fermentation	Enzymatic cellulose hydrolysis with or without <i>in-situ</i> cellulase production (batch production, continuous solid state fermentation, cellulase recycling); Separate hydrolysis and fermentation (SHF); Simultaneous saccharification and glucose fermentation (SSF); Simultaneous saccharification and co-fermentation (SSCF)
Final products and co-products processing	Lignin utilization (Co-generation, pyrolysis, enzymatic depolymerisation); Xylitol production from pentoses; Polymerisation of lactic acid (if lactic acid a fermentation product); Ethanol separation (fractional distillation, selective sorption); Ethanol dehydration (Molecular sieve separation, pervaporation, azeotropic distillation); Vinasses treatment (co-generation, methanisation, composting, land-filling)

integration and take advantage of fermentation organisms that must be tolerant to different operation temperatures and must be capable of using different substrates with high selectivity.

This paper discusses developments at Swiss Federal Institute of Technology Lausanne (EPFL) of a modular platform for integrated assessment (MPIA) for LCBR including logistics optimisation, process design and simulation, process economics and life cycle assessment (LCA).

Modelling Biochemical Pathways for Biorefineries and Lignocellulosic Ethanol Production: State-of-Art

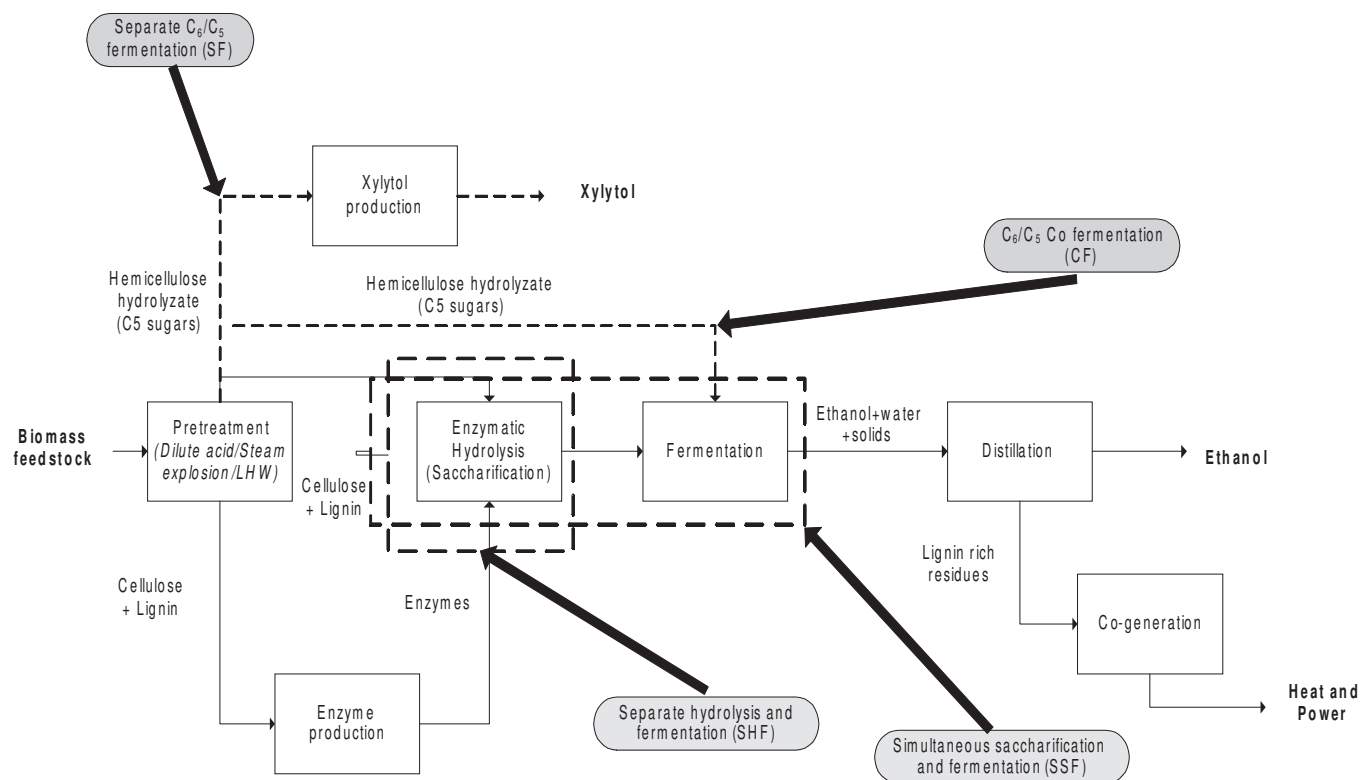
Upgrading and Diversification

In LCBR process, biomass conversion leads to a multifunctional system producing fuels, value added chemicals and possibly power generation (Fig. 2). There are multiple potentialities for a lignocellulosic or second generation biorefinery, in which biomass is fractionated after a pretreatment step into cellulose, hemicellulose and lignin. Cellulose could be hydrolysed into glucose and then fermented into ethanol or another bioproducts (lactic acid). Soluble hemicellulose could be fermented into ethanol or other co-products as xylitol, used as sweetener; in addition, products resulting from detoxification of hemicellulose hydrolysate, such as furan derivatives and phenolic compounds, could be used as building blocks for the production of fibers and resins. Lignin can be burned to produce steam or power, pyrolysed, or enzymatically depolymerised to produce

mono-aromatic compounds such as gallic and ferulic acids, building blocks for phenolic resins and fibers. Biorefinery concept offers an enormous potential for valorisation and long-term sustainability of biofuels production^{4,9-13}. Santos *et al*¹⁴ described experience of producing xylitol from sugarcane bagasse fibers. Gonçalves & Benar¹⁵ also reported hydroxymethylation and oxidation of organosolv lignins.

Supply-side Module

Supply logistics for bioenergy systems has been studied under a GIS based framework¹⁶⁻¹⁸. Production cost of ethanol from LB is quite sensitive to economy of scale^{7,8,19}. On the other hand, for processes dealing with high volumes of raw material and high capital costs, marginal changes in feedstock cost can make the difference^{16,17}. Therefore, in assessing economic viability of a LCBR, trade-off between plant size and raw material delivered cost must be taken into account. Delivered costs is sum of farm gate costs (costs incurred in feedstock handling at farm) and transport-related costs (loading and unloading cost, costs due to transportation from farm to plant gate, and administrative costs)¹⁷. Farm gate price may vary from one farm type to the other, depending on farm size and on agricultural practices (mechanisation, competition between uses, competitions between farms, income of farmers)¹⁸. NREL^{8,20} estimated farm gate price of corn stover for ethanol production by adding costs of fertilizer inputs (17%), baling and staging (60%) and a premium given to farmers (23%), calculated as a fixed profit per area unit representing likely threshold, above which



farmers would accept risk and added work of collecting and selling their residue. On the other hand, transport costs are directly related to plant size. In NREL study, transport costs represented 23% of total delivered cost, for a plant processing 2000 tons per day. Some studies^{16,17} linked bulky nature of LB with a significant impact in transportations costs underlining the importance of plant location and plant size. A GIS-based methodology¹⁷ to determine marginal price surfaces under several facility size scenarios was applied to potential switchgrass-to ethanol conversion facilities in Alabama (US). Using GIS, NREL and Oak Ridge National Laboratory (ORNL, US) developed a model to estimate energy and environmental flows and costs for collection and transportation of corn stover in the state of Iowa, accounting for soil erosion constraints^{8,21}. For this model, sustainable corn stover removal rate was estimated to 5 tons/ha for no-till practice and no crop rotation. It was estimated that 10 % of total farm area would correspond to these characteristics. EPFL¹⁸ developed a GIS-based decision support system (DSS) for selecting least-cost bioenergy locations when there is a significant variability in biomass

farm gate prices and when several bioenergy plants with a fixed capacity have to be placed in the region. Valorisation of agricultural residues represents an alternative to open-field burning strategies, which are increasingly discouraged due to air pollution and soil depletion. Crop residues (sugarcane harvesting residues^{22,23,24} and rice straw^{1,25}) are burned as a low-cost strategy to facilitate harvesting and avoid plant diseases if residues are left in the field. Softwood forest residues must also be correctly handled to improve forest health and reduce fire risks by using them as feedstock for ethanol production^{7,26}. Kim & Dale¹ estimated potential for bioethanol production (205 Gt) from rice straw (731 Tg) per year, and also estimated potential of ethanol production (51.3 Gt) from bagasse.

Process Design Aspects

Process design is core of an integrated assessment for LBCR and, in particular, a basic input for supply logistics and process economics evaluation as well as for environmental impact assessment (Fig. 3). NREL²⁷ has developed an Aspen Plus (Aspen Technology Inc.,

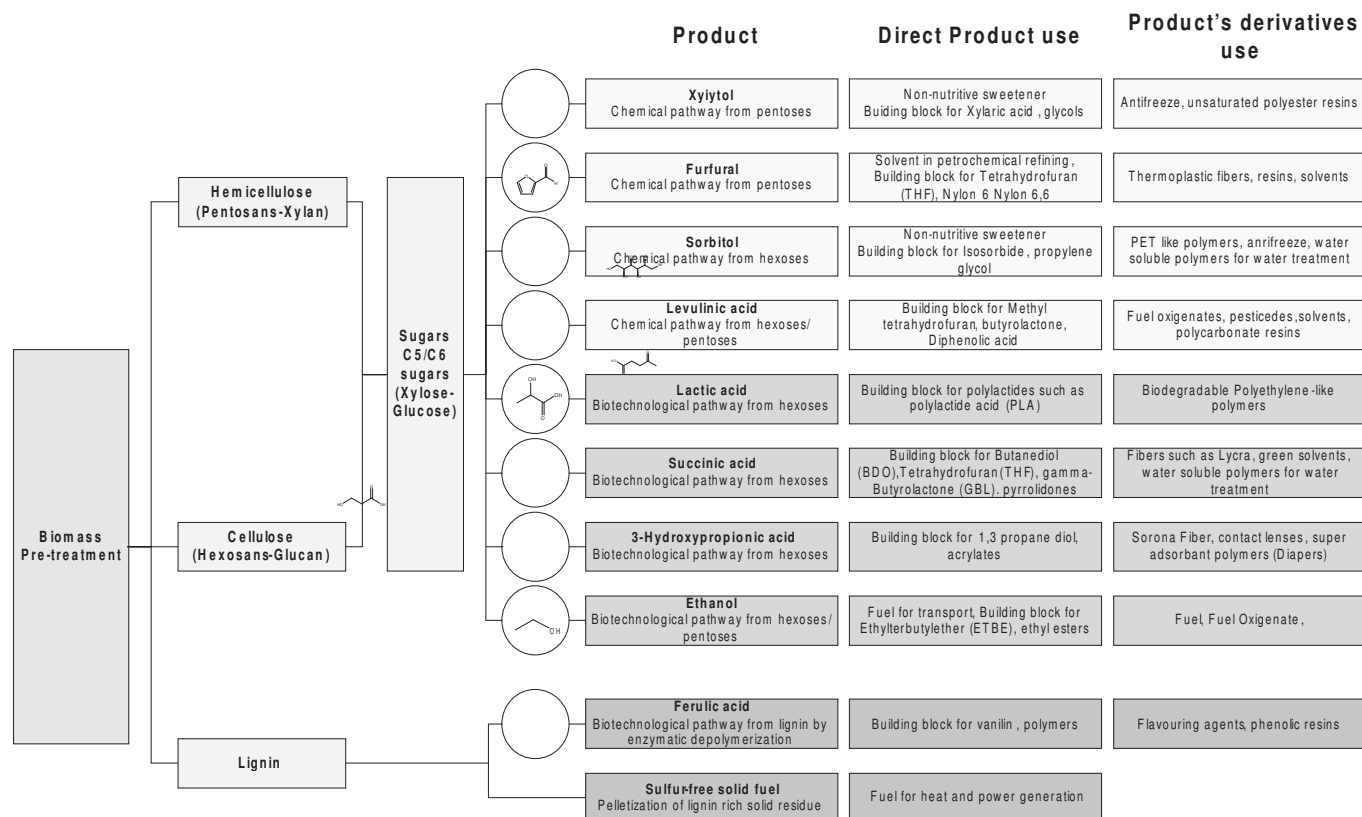


Fig. 2—Diversification panorama of LCBR pathways

USA) in-house database with thermodynamic and other physical properties specifically related to biomass for bioethanol production. Rigorous material and energy balances permit to evaluate technological options, represented by a particular flowsheet design, and obtain robust outputs regarding environmental impacts and economic viability, with a level of detail related to the stage of bioenergy project and its objectives (conceptual design, scale-up, direction of research, etc). Feedstock supply and composition (Table 2) are important issues that influence the choice of flowsheet design and overall pathway performance⁷.

Hardwoods are, in general less recalcitrant to pretreatment than softwoods, because their hemicelluloses are composed of highly acetylated xylans and acetate groups that rapidly hydrolyses into acetic acid in water, encouraging autohydrolysis of sugar polymers. In that sense, hardwoods are more susceptible than softwoods to autohydrolysis-low-severity methods^{29,30}. Hardwoods also present lower contents of readily fermentable sugars (C6), as do agricultural residues and herbaceous crops. This implies: 1) Selection

of a pretreatment method that encourages hemicellulose recovery while maintaining acceptable rates of cellulose hydrolysis and low levels of soluble inhibitors; and 2) Selection of downstream strategies aimed at valorisation of C5 and C6 sugars.

Thus, one could obtain valuable information on process design trade-offs if process simulator dynamically responds to changes in inflow rate and feedstock compositions taking appropriate flowsheeting choices, while maintaining thermodynamic and individual equipment sizing consistency. Kinetic models predicting conversions can be of great help to support dynamics and semi-automation of process simulation depending on feedstock characteristics and operational conditions.

Pretreatment Kinetics

A common approach to tackle kinetics of pretreatment consists of using a parameter relating reaction conditions into a single reaction ordinate to facilitate comparisons between different pretreatment methods and to use it in predictive models of sugar recovery and yield of enzymatic hydrolysis^{30,31}. Severity factor³², R_0 , for

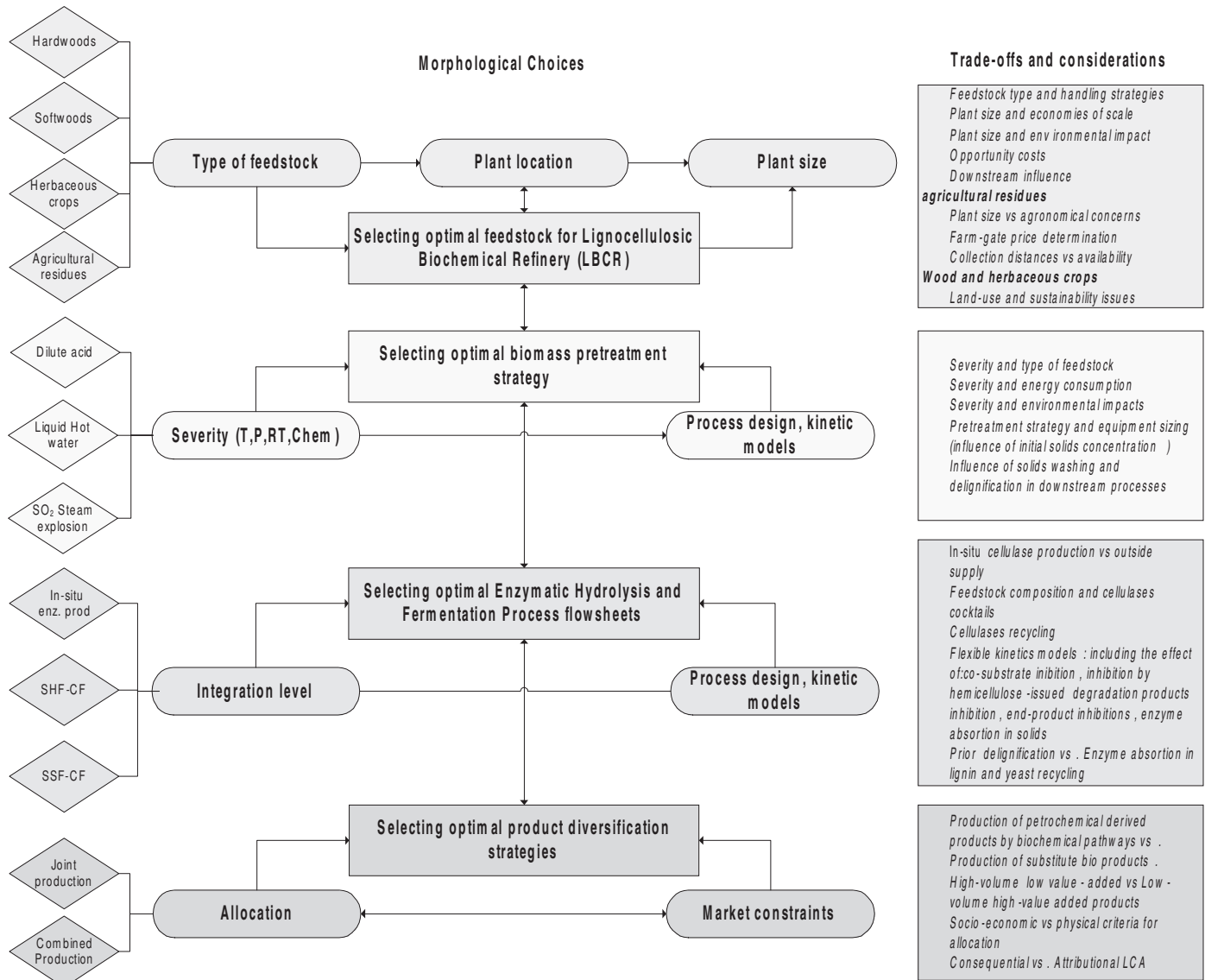


Fig. 3—Potential trade-offs related to supply logistics and process design

biomass pretreatment is a trade-off between reaction temperature and residence time in an approximation to Arrhenius equation. Bouchard *et al*³³ related R_0 to evolution of water soluble hemicellulosic fractions (pentosans and acetyl groups), and of compounds derived from lignin (methoxyl groups and polyphenolics).

$$R_0 = t * e^{(T_r - T_b / \omega)} \quad \dots(1)$$

$$\omega = \frac{T_f^2 R}{E_a} \quad \dots(2)$$

where, t= time (min), Tr= reaction temperature, Tb= base temperature, usually set to 100°C, ω = constant, T_f =

Floor temperature, R=Universal gas constant, and E_a =Activation energy.

To better fit for experimental data of acid catalysed steam pretreatment or organosolv pretreatment, Chum *et al*³⁴ proposed combined severity factor (CS), which also assumes a first order rate contribution from acid catalyst. Tengborg *et al*²⁹ used the combined severity factor to describe pretreatment of softwood with different degrees of H₂SO₄ impregnation in production of ethanol at different reaction conditions and related this parameter to yields of fermentable sugars and ethanol.

$$CS = \log(R_0) - pH \quad \dots(3)$$

Table 2—Usual composition of common type of feedstock

Feedstock	Hardwood (yellow poplar) ⁷	Softwood (pine) ²⁸	Herbaceous crops (switchgrass) ²⁸	Agricultural residues (corn stover) ⁸
Cellulose (Glucan C6)	42.4	44.55	31.98	37.4
Hemicellulose	21.5	21.89	25.18	27.6
Xylan C5	18.1	6.3	21.09	21.1
Arabinan C5	0.5	1.6	2.84	2.9
Mannan C6	2.9	11.43	0.3	1.6
Galactan C6	0	2.56	0.95	2
Acetate	4.6	2.67	1.21	2.9
Lignin	26.6	27.67	18.13	18
Ash	1	0.32	5.95	5.2
Other	3.9	2.88	17.54	8.9

where, pH= pH at reaction conditions.

Hemicellulose solubilisation kinetics has been the focus of various studies for dilute acid pretreatment³⁵ and for autohydrolysis pretreatments³⁶⁻³⁸. In general, these kinds of model are based on assumptions such as pseudo-homogeneous conditions, first order kinetics and Arrhenius-type dependence of temperature. Jacobsen & Wyman³⁶ contested adequacy of batch-test based-homogeneous-first order kinetic models, which assume direct conversion of hemicellulose into sugar monomers. Cannetieri *et al*³⁵, though used pseudo-homogeneous kinetics to model dilute acid hydrolysis of forest residues for simplicity reasons, recognised that heterogeneous models are a better representation of real conditions and found consistent kinetic constants following Arrhenius theory describing hemicellulose degradation into monomeric sugars and degradation products such as acetic acid, furfural and 5-hydroxymethyl furfural (from C6 sugars). Oligomeric intermediates become important in biorefinery developments that envision valorisation of oligosaccharides in food and pharmaceutical industries/^{37,38}. Nabarlitz *et al*³⁷ developed and validated a model for kinetics of xylan autohydrolysis with experimental results from pretreated corncobs. Carvalho *et al*³⁸ tested different sequential pseudo-homogeneous first-order kinetic models for brewery's spent grain autohydrolysis taking into account hydrolysis of xylan and arabinan and xylose dehydration to furfural.

Saccharification and Fermentation Kinetics

A kinetic model³⁹ for simultaneous saccharification and fermentation (SSF) should predict substrate conversion, with reasonable accuracy over a significant

range of substrate concentration, cellulase loadings, reaction time and substrate conversion. Kadam *et al*⁴⁰ developed a kinetic model for enzymatic saccharification, based on corn stover saccharification but intended to be used in a general way for *in silico* process optimisation. The model consisted of three hydrolysis reactions (2 heterogeneous reactions for cellulose breakdown to cellobiose and glucose and 1 homogeneous reaction for hydrolysing cellobiose to glucose). Heterogeneous kinetics took into account biochemistry of enzymatic hydrolysis, absorption and desorption phenomena onto and of cellulose and lignin substrates, substrate reactivity as well as thermal effects and end-product inhibition. This model takes into account, additionally, fermentation by *Saccharomyces cerevisiae* and ethanol inhibition. All of these models follow Michaelis-Menten type of kinetics for hydrolysis of soluble cellobiose to glucose, use Langmuir competitive absorption models for heterogeneous cellulose-lignin system; use pseudo first-order constants fitted with Monod kinetics for glucose and/or pentose fermentation and Arrhenius model for temperature dependence. Regarding specific case of co-fermentation, Leksawasdi *et al*⁴¹ presented a model for glucose and xylose fermentation taking into account substrate limitation, substrate inhibition and product (ethanol) inhibition.

Cellulase production represents an important share of ethanol production costs^{7,8}. In 1999, NREL's model of hardwood-to-ethanol pathway⁷, *in-situ* cellulase production by submerged fermentation (SmF) from aerobic fungus *Trichoderma reesei* was envisioned. In 2002, in corn stover-to-ethanol model⁸, cellulase off-site

production was considered due to cost considerations. Installed capital operating costs associated to *in-situ* production were about US\$0.079 per liter ethanol, whereas a cost of US\$0.026 per liter of ethanol was estimated for enzyme delivered to the plant from a local enzyme facility. However, solid-state fermentation could imply lower energy requirements and lesser wastewater generation⁴², becoming an interesting alternative to reduce costs of *in-situ* production. Coupling of kinetics models with process simulation can be a useful tool to improve economics and sustainability of bioconversion processes. For SmF processes, microorganism growth is often modeled following variants of Monod kinetics and enzyme production with variants of Leudeking pirt model^{43,44}. On the other hand, when developing solid-state kinetics, difficulty lies in separation of microbial biomass and substrate and therefore classical method for biomass growth determination are not suitable making necessary an adequate correlation with factors such as CO_2 production and O_2 consumption⁴⁴. Using these control variables, a few attempts have been made to model kinetics of oxygen consumption and temperature dependence of solid-state fermentation systems in general⁴⁴⁻⁴⁶.

Another way for enzyme-related costs reduction is an adequate recycling scheme of cellulases for enzymatic hydrolysis stage. A kinetic model for enzymatic hydrolysis must take into account the competition for cellulase absorption between lignin and cellulose^{39,40,47}. This competition can be a bottleneck for cellulase recycling if no previous delignification step is implemented. Addition of surfactants can be useful to decrease non-productive binding of cellulases to lignin⁴⁷.

Process design of upgrading alternatives of bioconversion of lignocellulosics processes into biorefineries can also be enhanced by adequate kinetics models. Lactic acid, an alternative to ethanol as a fermentation product, is a building block for polylactates, biodegradable polymers representing a potential substitute for polyethylene sharing with it similar physical properties such strength and elongation to break^{4,48-50}. Luo *et al*⁴⁸ pointed out that using SSF for lactic acid production, enzymatic hydrolysis and lactic acid fermentation work at similar optimal conditions of temperature and pH for a theoretical yield of 100% of lactic acid. Kinetic models for cellulose symbiotic breakdown and for glucose consumption were developed taking into account competitive absorption with lignin. Xylitol, mostly produced from chemical pathways but

could be alternatively produced via fermentation of xyloses⁵¹⁻⁵³, is another potential biorefinery's output resulting from C5 hemicellulose. Xylitol is mainly used as a sweetener with anticariogenic properties but can also be used as plasticizer for hardwood xylans^{52,54}. Rivas *et al*⁵² estimated kinetic parameters and developed carbon material and bioenergetic balances for xylitol production from corncobs using yeasts.

Environmental Impact

LCA has been used for environmental impact evaluation of lignocellulosic ethanol production and can be a useful tool to evaluate LBCR in general^{21,55-61}. LCA for biorefineries have been restricted mainly to diversification schemes of existing first generation food crops-to-biofuels pathways (wet mill cereal-to-ethanol pathway^{58,62-64} or soybean oil valorisation chain⁶⁵). Environmental impacts of LBCRs have only been estimated for pathways with a low degree of product diversification delivering ethanol and energy from lignin-rich residues^{21,55,56,59-61}. However, there is a huge potential for large-scale production of bulk chemicals from dedicated lignocellulosic crops or agricultural residues to directly replace or at least to offer similar functions than its fossil-based counterparts. LCAs for highly diversified biorefineries must be restrained to generic approaches due to limitations in process data availability and uncertainty in technological developments. Hermann *et al*⁶⁶ performed LCA for an extended group of biochemicals assuming that yield for sugar-based bioprocesses was independent of the type of sugar and therefore from the type of feedstock. In general, when evaluating environmental performance of a LBCR by means of a LCA, there are some methodological issues, inherent to methodology. One of these issues, and also a main weakness of a LCA of a multi-product system, is the problem of allocation or the way in which environmental burdens are distributed between the multiple outputs of the biorefinery. Complexity of the allocation problem increases in the case of a highly diversified biorefinery -one producing various commodity chemicals and energy. Most of the products envisioned for a LBCR have no formal or established markets^{4,67}. In occasions, these new products are substitutes for petrochemical commodities providing also additional or slightly different functions hampering by this fact the application of economic or substitution approaches. Multifunctionality could also make difficult an appropriate value attribution to perform an allocation based on physical

property such as energy contents, mass or carbon contents. In addition, a system of this kind will probably present a highly dynamic nature due to supply-demand evolution linked to changes in production priorities and investment strategies. In that sense, consequential variants to conventional LCA methodology can be an option to deal with this issue. A consequential LCA can be defined, in contrast to an attributional LCA as a methodology aimed at description of how environmentally relevant physical flows to and from technosphere will change in response to possible changes in the life cycle including unit processes that are significantly affected whether they are inside or outside the life cycle⁶⁸. A LCA framework coupled with partial equilibrium microeconomic models, used by Freire *et al*⁶⁹ to optimise resource allocation and policy scenarios for biofuel introduction in France, offers possibilities to be extended to dynamic behaviour assessment of biorefineries.

Another weakness of LCA is related to linearity that governs input/output relations in that method. Non-linearity of production functions, particularly in the case of highly diversified biorefinery processes, is common rule. Mathematical relationships describing a process are, in general, dynamic and non-linear and this may be taken into account in LCA practice depending on assessment objectives, data availability, and availability of dedicated software, and accuracy and robustness constraints⁷⁰. In that sense, process simulators can help to evaluate to which extent the assumption of linearity for a particular production function is consistent with reality. Moreover, coupling of rigorous process design and LCA has been proposed to optimise production process according to environmental and economic criteria⁷¹⁻⁷⁴. Since 1970's oil crisis, objectives in process design have shifted first to incorporate energy savings into chemical process and then to increasingly include environmental and sustainability concerns. Cano Ruiz & McRae⁷¹ reviewed methodological issues and research needs related to integration of environmental concerns including LCA as a framework to estimate environmental impacts as well as, for process synthesis, hierarchical design approaches, expert systems and other artificial intelligence approaches. Azapagic⁷² recommended inclusion of LCA in the first stages of process design using a mixed integer linear programming (MILP) multi-objective optimisation in order to identify a set of Pareto-optimum solutions for improved design. Chen *et al*⁷³ presented results of a multi-objective optimisation of a volatile organic chemicals (VOC) recovery process and a heat exchanger network

(HEN), and coupled process simulation with HYSYS (Aspen Technology Inc., USA) with LCA. Environmental Fate and Risk assessment Tool (EFRAT) was used for impact assessment and annualised capital and operating costs were used as economic performance indicators. Optimisation was carried out through Analytical Hierarchy Process (AHP). Quintero *et al*⁷⁵ followed a similar approach and applied to first generation ethanol production pathways. Most of the emphasis in multi-objective optimisation approaches using LCA has been put in process design aspects. However, supply logistic plays an important role in an integrated assessment of LCBR and in bioprocesses in general. Hugo & Pistikopoulos⁷⁴ developed a MILP combining classical plant location and capacity expansion problem with the concepts of LCA and multi-enterprise supply chain management. They used Eco-indicator 99 as aggregation factor for impact assessment and conventional net present value (NPV) as economic performance measure of vinyl chloride monomer (VCM) and ethylene glycol (EG) supply chain. Complexity of overall problem requires effective optimization algorithms for reducing computational burdens and assuring convergence. Steffens *et al.*⁷⁶ illustrated potentialities for application in bioprocesses of *Jacaranda* system, a Java written application, useful for multicriteria process synthesis. Application uses discretisation to convert a mixed integer non-linear programming into a graph generation and search problem. Algorithm proved able to generate list of N-best flowsheets in a reasonable computational time for a penicillin production process restricted to the manufacturing stage. While *et al*⁷⁷ developed a multi-objective evolutionary algorithm for mineral processing optimisation and process design. Jan *et al*⁷⁸ developed a new hybrid Genetic/Quadratic search algorithm (GQSA), coded in MATLAB[®] Version 6.0, to optimise plant economics when a process simulator models the plant. They took advantage of Active X components in Aspen Plus (Aspen Technology Inc., USA).

Process Economics

Economic viability of lignocellulosic-based bioprocesses has been studied through detailed process design data in order to optimise research direction^{7,8,79-82}. Nguyen & Saddler⁷⁹ developed a process simulation model using Lotus 123 (IBM, USA) to evaluate technical and economic feasibility of a plant processing 500 tons of aspen wood per day to produce ethanol, using SO₂ catalysed steam explosion, delignification and separate

pentoses fermentation. Feedstock, enzyme production, efficiency of cellulose hydrolysis, ethanol yield from xyloses, efficiency of delignification and credit attributed to lignin as fuel co-product were major contributors to production cost of ethanol from wood. NREL models from 1999⁷ and 2002⁸ established process design models and cost estimates for hardwood-to-ethanol and corn stover-to-ethanol pathways, respectively. Aspen Plus (Aspen Technology Inc., USA) process simulator was used to estimate material and energy balances. Capital costs and equipment sizing were carried out through vendor quotes and estimations from ICARUS Process Evaluator (Aspen Technology Inc., USA). In 2002 version, NREL changed base case feedstock from yellow poplar to corn stover which was considered as a promising feedstock, and left behind SSF as well as *in-situ* enzyme production in order to better portray the state of research. For this pathway, they calculated minimum selling price (MESP) of ethanol in US\$0.283 per liter using a Discounted Cash Flow (DCF) model and Montecarlo simulation. Using a similar approach, other researchers^{81,83} studied trade-offs for softwood-to-ethanol pathway, including effect on ethanol production costs of enzyme costs, substrate loading in SSF and SHF modes, and various schemes of stream recirculation and steam pre-treatment configurations. In a previous work of EPFL⁸⁰, different alternatives of sweet sorghum valorisation, including among others co-generation and ethanol production from sweet sorghum bagasse, were compared through process simulation with Aspen Plus and economic performance analysis. In the framework of Biomass Refining Consortium for Applied Fundamentals (CAFI) UDA Initiative for Future Agriculture and Food Systems (IFAFS)⁸², techno-economic models for five biomass pretreatments (dilute acid, hot water, AFEX, ammonia recycle percolation (ARP) and lime) were developed and inserted into 2002 NREL model. In general, all of these studies use process simulation and DCF models to assess different technological variants. None of these variants include a diversification strategy to produce bulk chemicals from sugars or a different alternative to fuel use for the lignin-rich residue.

Until now, all techno-economic evaluations of lignocellulosics bioconversion processes have used DCF models, which rely on economic performance measures such as NPV, Internal Rate of return (IRR) and Discounted Payback Period (DPP). All of them can be used to compare alternative investments or projects of

energy efficiency and renewable energy technologies⁸⁴. However, NPV has been traditionally viewed as a more reliable measure of economic performance than the IRR and the DPP^{85,86}. When using IRR certain cash flows can generate NPV=0 at two different discount rates, or can show NPV of project increasing as discount rate increases, contrary to normal relationship between NPV and discount rates⁸⁵. DPP presents also inconveniences such as the fact that it only accepts projects that payback in desired time frame ignoring later year cash flows and present value of these future cash flows⁸⁵. However, traditional NPV analysis can also lead to underestimations of benefits associated with a project due to the implicit assumption that companies holds its assets passively, ignoring management flexibility and the intangible advantages linked to discretionary investment opportunities⁸⁵⁻⁸⁷. A biorefinery can be by nature a highly dynamic investment project. Biorefineries are multi-output systems characterised by implicit technological and market uncertainties, in which production priorities and investment decisions will be possibly much diversified across time. It is the case of lignocellulosics-to-ethanol production pathways, which are expected to be gradually upgraded into bulk-chemicals-and-fuels production pathways. In future, substantial cost reductions could be attained for this pathway regarding control of fermentation inhibition, lactic acid recovery from fermentation broth and control of molecular weight and properties of final polymers^{4,53,88}. Switching of dedicated crops to agricultural or even industrial residues also represents an investment opportunity that could add value to the project. To overcome limitations of conventional NPV when assessing the merit of a project like that of a biorefinery, some methodologies are proposed such as adjusted present value⁸⁶, which includes impact of dynamic decision making and the value of real options. The real options for an investment project can be classified into six categories based upon the type of flexibility provided⁸⁶: 1) option to defer; 2) option for staged investments (the project is broken into discrete phases and the next phase is not started until current phase has been completed); 3) Option to change scale (project can be expanded, contracted or shut down and restarted depending on market conditions); 4) option to abandon (also related to market conditions); 5) option to switch (option to change either input or output of the project, can be related to change in feedstock and/or biorefineries diversification); 6) option to grow (option to make investments based on future growth value even

if there is a negative traditional net present value, related to uncertainty in technological and market development of certain biorefinery products). In IFAFS project⁸², little differentiation was found between economic performances of biomass pretreatment strategies varying from low cost to capital intensive options. However, study recognised that it was not completely fair to make economic comparisons between pretreatment options given the different stage of development between them. The study recommended using real options analysis to adjust DFC to differences in state of development, complexity, reliability, differing potential for creating environmental and safety uses, etc.

In the framework of biomass conversion, opportunity costs can be defined as the costs forgone by choosing one option of biomass valorisation over an alternative one that may be equally desired. In EPFL study⁸⁰, in which alternative uses were considered, including ethanol production for sorghum juice and sorghum bagasse, an opportunity cost approach was coupled to DCF models. A great sensitivity to ethanol and sugar prices was found, which resulted in the necessity of flexible installations capable of switching of production objective according to demand. Alternative use of biomass was also evaluated for excess sugarcane bagasse utilisation⁸⁹. Proposed model was called “Environmental System Optimization” under a LCA framework and using weighting factors for economic and environmental objectives. Instead of using process simulation inputs, their model relied on reported values and on SimaPro V5.1 (Pré Consultants, the Netherlands), which uses built-in Ecoinvent (Swiss Centre for Life Cycle Inventories, Switzerland) databases. After determining environmental impacts of two options, it was concluded that utilising excess bagasse as feedstock was desirable for ethanol production.

Modular Platform for Integrated Assessment (MPIA) of LCBRs

Modular Platform for Integrated Assessment (MPIA) of LCBRs evaluates LCBRs from an environmental and techno-economic point of view. Platform includes 4 modules (logistics optimisation, process design and simulation, process economics and LCA) (Fig. 4). Modules presented here are deeply interconnected. Some of the modules will be partially automated in order to assess composition and scale issues. Platform will provide a DSS for designing and evaluation consistent LCBRs following a holistic approach. Ongoing research at EPFL

is aimed at development of multi-criteria optimisation approaches including evolutionary algorithms, hierarchical design approaches and other methods of structured thinking, expert systems and artificial intelligence approaches.

Supply-side Module

EPFL GIS-based DSS for selecting least-cost bioenergy locations is currently being expanded to the specific case of lignocellulosic bioethanol plants including an environmental objective function. This module aims to determine biomass potential to satisfy a given bioethanol demand based on political, social, economical, environmental, technological, and agro-ecological constraints and to determine optimal plant size and logistic configurations in order to reduce operational costs and environmental burdens. Information provided by this module is intended to be used along with LCA and automated process simulation tools.

Process Design Module

This module is based in automation of Aspen Plus process simulator to investigate effects of plant size and feedstock type and composition throughout the whole life cycle of LCBR. Automation strategies are currently being developed at EPFL by means of external automation software such as MATLAB and Visual Basic for applications (Microsoft Corp, USA) taking advantage of Active X components in Aspen Plus. These consider development of user customised reactor units in Aspen Plus incorporating kinetic models for pretreatment, saccharification and fermentation steps. Kinetic models are intended, when possible, to take into account heterogeneity, substrate limitation, end-product inhibition, as well as inhibition from organic compounds resulting from biomass pretreatment. Selection of pretreatment methods and configurations will depend on feedstock type and downstream integration and diversification choices, using C5 and C6 sugar yields after pretreatment as parameters. Platform is being developed through lignocellulosic-to-ethanol pathways but will be extended to more diversified pathways after validation and tuning with these backbone pathways.

Environmental Impact Assessment Module

LCA methodology was chosen to determine environmental impacts related to different LCBRs. This impact assessment will be restricted in initial developments to estimate greenhouse gas (GHG)

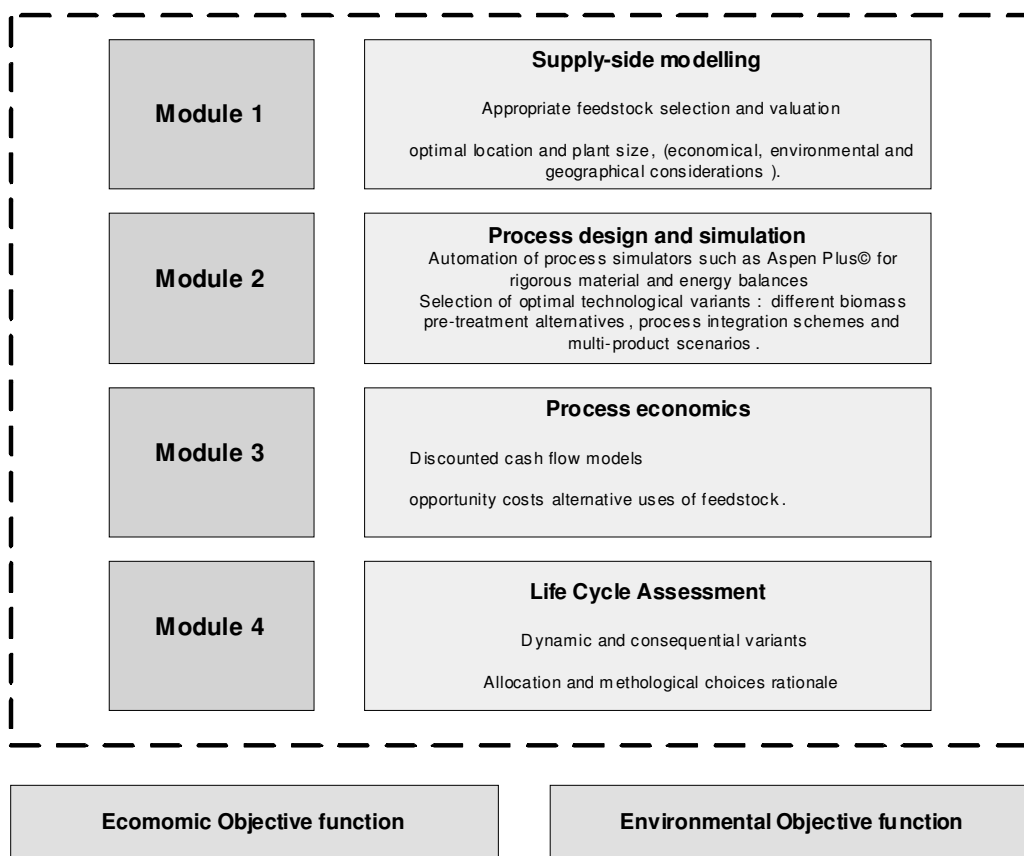


Fig. 4—Modular platform for integrated assessment (MPIA) of lignocellulosic biorefineries (LCBR)

balances using Global Warming Potential (GWP 100a) (IPCC, 2003) and energy consumption using non-Renewable cumulative energy demand (CED). This is done because other weight-based aggregation methods such as Eco-indicator 99 can cause too much noise to platform outputs due to the introduction of subjectivity. Information from Process Design Module and Process Economics Module consisting in mass and energy balances can be used to give light to some LCA methodological controversies such as non-linearity of production function and allocation problem. These two issues can be of particular importance for highly diversified pathways.

Process Economics Module

This model couples LCA outputs to DCF models in order to select optimum LCBR flowsheets according to environmental and techno-economic criteria. Ongoing research is devoted to find alternatives valuation methodologies, such as adjusted present value and real options analysis, in order to adequately account for highly dynamic nature of a multi-output system such as a

lignocellulosic biorefinery, characterised by significant technologic and market uncertainties. Mutually exclusive uses of biomass feedstock will be considered for each pathway and opportunity costs will be accounted for.

Conclusions

Conceptual design of MPIA was discussed drawing a road map for its development and presenting ongoing research at EPFL. Challenges regarding ethanol production from lignocellulosic residues and upgrading of this pathway into a biochemical refinery include supply logistics optimisation, optimisation and selection of adequate biomass pretreatment methods, improved integration of bioconversion processes, and development of sound pathways for the production of commodity chemicals. A meaningful assessment of this kind of pathway must integrate a maximum of information regarding the whole life cycle of biorefinery products. Therefore, MPIA must include GIS-models, semi-automated process design simulations incorporating kinetic models for chemical and biotechnological process, LCA and DCF models taking into account the highly

dynamic and flexible nature of a multi-output system such as a lignocellulosic biorefinery. However, a decision support tool like this must remain flexible and user friendly and therefore a trade-off must be made between complexity and system limits.

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