Model-based Optimization of Microalgal Biorefineries by Dynamic Flux Balance Analysis (DFBA)

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Photosynthetic microorganisms such as cyanobacteria and microalgae are innovative cell factories for sustainable production of valuable products from renewable feedstocks. The broad scope of application for microalgal compounds includes the feed, food, bioenergy and biochemical sector.

The content of high-value products, such as carotenoids or polyunsaturated fatty acids, in the biomass is typically low and a large fraction of residual biomass remains unused. In contrast, the economic feasibility is often difficult to achieve because of energy and cost-intensive harvesting and extraction steps. Therefore, microalgal process design requires tailor-made downstream processing strategies and a biorefinery approach to valorize most of the biomass fractions.

In this contribution, we present a model-based approach that quantitatively describes various biomass fractions in the green alga Dunaliella salina, the most important organism for industrial beta-carotene production. This approach makes use of Dynamic Flux Balance Analysis (DFBA). The underlying metabolic network is based on the well-established genome-scale reconstruction of the model organism Chlamydomonas reinhardtii. The DFBA model provides a detailed mechanistic description of the intracellular stoichiometry and metabolite accumulation in combination with changes in the extracellular environment. This is used to formulate a structured dynamic model that predicts growth, metabolic activity and biomass composition in a dynamic bioreactor environment. We demonstrate that the developed DFBA model correctly predicts the growth rate and the production rates of valuable metabolic products such as pigments and lipids under different light and nutrient conditions that match well with our experimental findings. As an example, in an experimentally validated fed-batch optimization study we increased the biomass and the β-carotene density by factors of 2.5 and 2.1, respectively.

Our model can thus be used to design an optimal alga--based biorefinery and/or to improve performance of existing bioproduction processes for achieving an economic feasible overall process operation under the consideration of all essential up- and downstream steps.

Selection of optimally integrated biorefinery processes by early-stage design decision making approach

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Biorefineries are integrated processing facilities that convert biomass into value added products and energy, aiming maximization of the economic value of biomass while minimization of the waste streams. Lignocellulosic biorefineries are considered as the best alternative to promote the transition from a fossil fuel-based to a bio-based one for a sustainable development. The design of a biorefinery brings a significant number of challenges due to large number of processes available and possible products. It requires the use of advanced process synthesis and optimization methods to ensure that these systems are economically viable, energy efficient, have minimum environmental impact and realize the best use of the biomass resource. It is important to implement an algorithm that allows systematic generation and evaluation of biomass conversion chains and making comparison of the different pathways, ranking them according to different criteria. To achieve this, a methodology has been proposed to define systematically ordered set of solutions using mixed integer linear programming (MILP) models with integer cut constraints (ICC) [1]. In this study, we apply a systematic process design approach which adopts thermo-environomic optimization together with heat integration to assess the economic performance, environmental impact and energy requirement for several process options of both sugars (biochemical conversion) and syngas (thermochemical conversion) platforms to compare processes with output of different nature (energy services, valuable chemicals, fuels). A superstructure of different process models is developed and the heat recovery is represented by characterization of the process unit energy requirement 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. This methodology is fast and powerful and can be used as an early stage decision making tool.

Systematic Process Development of Integrated First and Second Generation Biorefineries

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Recently, the integration of different generation biorefineries has attracted attention, since the integrated scheme can contribute to a more economical design with lower environmental impacts than the stand-alone. Second generation technologies can be used to upgrade, rather than eliminate existing first generation plants, as they process different feedstock. But, to date, first and second generation processes have been integrated by the adoption of grassroots design methodologies, while, in reality, their coupling is far more complex. While first generation installations are nascent plants, still possible to amend and modify, second generation upgrades account for new technology and investment very flexible to adjust so that the upgrades are best. Furthermore, there is significant potential to exchange (by-)products and not only to integrate energy. Moreover, the processes may utilize common sections, like sharing the same fermentation and/ or dehydration section. That implies a retrofit problem that is much larger and complex than most conventional applications. This is why, the integration of different generation biorefineries is a combined grassroots–retrofit design problem that hides inner trade-offs and proves the deficiency of present-day practices in proposing realistic designs for such mixed design problems.

In this work, detailed designs of first and second generation ethanol production are developed in Aspen Plus® and validated by the industrial partner (CIMV Process™). The detailed models feed the mathematical models, developed in GAMS®. The model applies the methodology of grassroots integration on second and retrofit integration on first generation technology, following the transhipment analysis. Preliminary results indicate a significant potential in internal trade-offs savings, both in operating and capital cost. Although a range of software tools exists for the simulation of processes, customization is usually required when more details are required. There are enough data to generate more precise models searching not only the optimum process but also the optimum equipment design. For complex problems, a single software tool may be insufficient. In that case, it is the interoperability of software can create a powerful.

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Production of sugar platforms from lignocellulosic biomass – Energy analysis and techno-economic comparison

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The use of lignocellulosic biomass for the production of biofuels and a variety of platform chemicals represents a step forward in the transition to a bio-based economy. Large chemical and food companies have begun to invest in the development of technologies that are able to provide a suitable sugar platform from a large variety of lignocellulosic feedstocks. In this work, a process model is developed (in Aspen Plus) which allows to determine the mass and energy balances of alternative processes for the conversion of lignocellulosic biomass into sugars. These sugars can, for example, be converted to ethanol as fuels in blends with gasoline or for the production of chemicals. Six processes are studied, i.e. (i) dilute acid (DA), (ii) liquid hot water (iii) steam explosion, (iv) ammonia fiber explosion (AFEX), (v) combined supercritical and subcritical hydrolysis, and (vi) Organosolv pretreatment. First, corn stover is studied in detail as model feedstocks, allowing to analyze the technical challenges of different biomass pretreatment technologies, including energy integration. The systems are considered as stand-alone plants producing syrup of 50% solids, containing both six-carbon and five-carbon sugars. Each system considers the combustion of solid lignin-rich residue for cogeneration. Since different types of crops and plant materials require specific types of pretreatment and since the availability of crops and crop residues differ by region, a range of feedstock-region-technology combinations are subsequently studied. A comparative analysis is performed for (i) US: corn stover/cobs, yellow poplar, arundo donax (ii) China: corn stover, wheat straw (iii) Brazil: sugarcane bagasse, corn stover (iv) India: rice straw, wheat straw, sugarcane bagasse, cotton straw, v) South East Asia: empty fruit bunch, vi) Europe: Pine, arundo donax, wheat straw. All alternatives are compared in terms of minimum sugars selling price (MSSP) which are also compared with the cost of sugars from food crops (sugarcane, sugar beet, wheat and corn) as traded on the world market.

Integrated Biomethanol Production

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The Mantua Chemical District is a Site of National (and European) Interest (SIN). Mantua's SIN uses about 150 kt/y of methanol to produce formaldehyde, an important intermediate in several chemical processes. Nowadays the oil refinery is off and the industrial network is deeply suffering from it, with the authorities at all the levels (town, province, region, and ministry) that are moving fast to convert the SIN into a biorefinery.

This paper illustrates the studies and results of the funded project BioMAN to transform the Mantua SIN into a lignocellulosic biorefinery. Among different production routes, the production of methanol was initially investigated for its integration within the SIN complex.

In this paper, an energy integration scheme is proposed, aiming to further develop the combined production of fuel and energy:

- An initial scheme is taken as a base case for fuel production. The scheme can be adapted in such a way that different fuel/energy outputs are possible.

- Such adaptations are done by inserting elements such as a turbine or a heat exchanger into the existing initial scheme.

- The surplus energy in form of steam or electricity can be sent to the grid, which translates into additional income.

Among expected contributions of such findings are, first, the directive guidelines for the revamping of such site and, second, development of a conceptual framework for the application of optimization techniques as energy integration tools.

Optimising biomass-based energy supply chains for sustainable mobility

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The identification of alternative and sustainable energy sources has been one of the fundamental research goals of the last two decades, and the transport sector plays a key role in this challenge. Electric cars and biofuel fed vehicles may contribute to tackle this formidable issue. According to this perspective, a multi-echelon supply chain is here investigated considering biomass cultivation, transport, conversion into bioethanol and/or bioelectricity, distribution and final usage in alternative bifuel (ethanol and petrol) and electric vehicles. Multiperiod and spatially explicit features are introduced in a Mixed Integer Linear Programming (MILP) modeling framework where economic (in terms of Net Present Value) and environmental (in terms of Greenhouse Gases emissions) objectives are simultaneously taken into account. On the one hand, both the financial performance of the production supply chain and the economics of vehicle utilisation by end user are simultaneously taken into account and optimised for a strategic assessment of biomass exploitation. On the other hand, the environmental performance is evaluated by considering the impact of each single life cycle stage and also incorporating the potential consequences related to indirect Land Use Change (iLUC). The first and second generation bioethanol production supply chain is matched with biopower production technologies, while both corn grain and stover are considered as biomass sources to produce either ethanol and/or electricity. Site location and scale, logistic infrastructure definition (biomass or bioethanol transport) and end user demand evolution for alternative fuel vehicles (bifuel or electric vehicles) are simultaneously incorporated within the optimisation model. All simulation studies will show that both bifuel and electric vehicles are needed for complying with the market demand and results will demonstrate the efficacy of the methodology at providing stakeholders with a quantitative tool to optimise the economic and environmental performance of different supply chain configurations.

Rigorous optimization-based design of energetically intensified distillation processes for the separation of non-ideal mixtures

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There is a permanent interest in improving energy efficiency and economic performance of industrial processes. Especially conventional distillation processes, which are still widely applied in chemical processes, suffer from low thermodynamic efficiency, offering large potential for improvements in terms of energy savings [1]. Therefore, various approaches to heat integration, thermal coupling and heat pumps have been proposed in order to improve energy efficiency of distillation processes. However, they are rarely compared in a single study.

Current approaches for screening these configurations rely on shortcut methods, like the Fenske-Underwood-Gilliland method, in order to determine the most suitable options which are verified by means of rigorous simulation [2]. These approaches are limited in two ways. While shortcut methods like the Fenske-Underwood-Gilliland method are limited in applicability and accuracy by the underlying assumptions of constant molar overflow and constant relative volatilities, rigorous simulation of thermally coupled configurations is complicated by the absence of readily available models in commercial simulation software. Dividing wall columns (DWC) usually have to be represented by complex configurations of available models for standard columns [3].

To facilitate a fast and reliable identification of energy and cost optimal process configurations for the separation of non-ideal mixtures, an efficient optimization-based method is proposed. The method relies on a superstructure approach including rigorous thermodynamic models for equilibrium and enthalpy computations [4]. Optimal designs are determined on the basis of the total annualized costs (TAC), considering investment and operating costs. Based on a sequential approach, a multitude of different energetically intensified distillation processes are evaluated, including conventional heat integration, thermally coupled and DWCs, as well as vapor recompression. All configurations associated to one sequence of splits are initialized by means of the common column sequence. Subsequently the optimization of each energetically intensified configuration is performed by means of an automated adaption of the superstructure. All process options are optimized for minimum energy demand and TAC. Based on the application to the separation of a ternary non-ideal mixture, the benefits of such an efficient tool are illustrated for the analysis of varying problem specifications, such as feed composition and varying utility costs.

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Shortcut-based evaluation of energetically intensified distillation processes under uncertainty

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The majority of fluid separations in the chemical industry are still performed by means of distillation columns, accounting for about 40% of the total energy consumption in this industry [1]. Consequently, energetically intensifying these processes provides a huge potential for energy savings. While a variety of different options for heat integration, thermal coupling and heat pump configurations have been proposed to improve energy efficiency of distillation processes, the economically most attractive configuration needs to be determined for a final implementation. In order to increase the confidence in the performance evaluation, uncertainties in process relevant parameters should also be taken into account [2].

The resulting problem of identifying the most promising process variant consequently can be formulated as a multi-scenario optimization problem, assuming discrete sampling points for the uncertain parameters [3]. While it is possible to address such an optimization problem directly, considering non-ideal thermodynamics and detailed equilibrium-tray models, e.g. by means of a two-stage stochastic programming approach [4], such an approach is still limited in the number of configurations and uncertain parameters that can be considered.

In order to efficiently address this problem for a large set of process configurations and uncertain parameters, a systematic screening procedure by means of a full enumeration of all process variants and scenarios based on reliable shortcut methods is proposed. In order to account for non-ideal thermodynamic models, the rectification body method (RBM) [5] is integrated in an automated evaluation procedure for various configurations, including heat-integration between single columns, thermally coupled configurations and the application of vapor recompression, based on isentropic compression. For the separation of a mixture into three products 18 different configurations are considered. Each of these configurations is automatically evaluated for several hundred different scenarios, in order to address the uncertainty associated to feed compositions, utility costs and the thermodynamic model. Based on the full enumeration of all configurations and all resulting scenarios the most efficient configurations as well as the most relevant scenarios are identified, and can further be investigated by means of a rigorous optimization approach based on equilibrium-tray models. The application of the shortcut screening is demonstrated for two case studies.

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Process Network Flux Analysis for an Early Design Stage Evaluation of Biorefinery Processing Pathways

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Growing interest in the biomass value chain and in the potential of biofuels leads to a high number of proposed biorefinery concepts and reactions converting biomass into a variety of biofuels. The arising design decisions, like the selection of the most promising processing pathways, need to be addressed systematically already in the early design stage to successfully guide future research activities. Since data is scarce and does not suffice for detailed process design, screening methodologies are required to identify sustainable and economic pathways.

Existing superstructure approaches apply mass- and energy-based evaluation of possible processing pathways [1-2] using simple performance models based on either tedious simulation studies or extensive literature searches restricting them to process concepts with an existing detailed design. In contrast, novel reaction pathways can be evaluated by Reaction Network Flux Analysis (RNFA). This optimization-based screening tool relies on reaction data like stoichiometry and yield to rank the reaction performance of biorefinery pathways [3], but does not address feasibility and performance of separations.

Herein, RNFA is extended towards Process Network Flux Analysis (PNFA) covering additionally the separation of solvents and products. It is based on a thermodynamic feasibility check to select the most promising separation strategy and a shortcut calculation of its energy demand. The assessment optimizes the cumulative energy demand and the processing cost.

As case study, the novel PNFA methodology is applied for a process network of the gasoline biofuels ethanol, iso-butanol, 2-butanone, γ-valerolactone, ethyllevulinate and 2-butanol. The results show that the PNFA successfully identifies mass- and energy-related bottlenecks. The studied biofuels are ranked according to their process performance enabling an early stage screening of existing and novel processing pathways. In particular, iso-butanol and 2-butanone are identified as most promising fuels beyond ethanol. 2-butanol can be ruled out as a pure-component fuel due to a lack in selectivity.

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Computer-Aided Molecular Design using process shortcut models and COSMO-RS

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Suitable solvents in process design can be identified using Computer-Aided Molecular Design (CAMD) methods [1]. CAMD inverts property prediction by designing molecules to meet a certain property target. The success of CAMD depends critically on two elements: An accurate property prediction method and sound property target. Previous work relied mostly on thermodynamic group contribution models (e.g., UNIFAC) and heuristic guidelines to define property targets.

In this work, we present a novel approach for Computer-Aided Molecular Design integrating state-of-the-art quantum-chemistry-based property prediction and the rigorous evaluation of the design based on a process-level assessment. The COSMO-CAMD framework is presented employing the property prediction method COSMO-RS [2] which found a successful compromise between accuracy of quantum-level predictions and computation effort. In order to overcome simplified solvent property targets such as partition coefficients of the solute in infinite dilution, the COSMO-CAMD framework is extended to optimize the molecular structure based on solvent's process performance. For this purpose, thermodynamic accurate process shortcut models [3] are employed. The shortcut models provide insights about extraction efficiency and minimum energy demand for separation. Thus, solvents are optimized based on process performance as objective function and tailored to real process flowsheets.

The resulting framework is applied to a hybrid extraction process taking into account extraction and distillation. Results show that solvents designed by the framework enhance solvent extraction performance and reduce energy demand compared to existing benchmark processes.

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Synthesis and Optimization of Processing Paths for Specialty Chemicals in Microalgae Biorefineries

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Microalgae as a source of biomass have been recently gaining ground especially due to the wide range of products they can offer. Thus, biorefineries capitalizing on this particular biomass are worth exploring not only from an experimental, but also from a conceptual point of view. The study pays attention to the valorization of specialty chemicals and attempts to address the limitations involved in the field of microalgae biorefineries. The selection of suitable technologies in addition to the identification of the product portfolio compose the elementary challenges amplified by the presence of competitive chemistries and the need for multi-product plants to ensure sustainability.

The methodology developed follows the combinatorial use of a superstructure and mathematical techniques to simultaneously screen and evaluate potential paths for the extraction of desired products. The problem is formulated starting with a set of feedstocks f that can be converted either to intermediates i or to final products p by the use of processes t. For feedstocks, intermediates and products the prices are known, whereas for the technologies yields and capital costs are known. The selection of processes and product portfolios are treated as degrees of freedom. In order to form all the available options, a superstructure is developed involving conceptual feedstocks, processes, intermediate mixtures or fractions and products. This is a crucial point, especially in the case of microalgae biorefineries, since establishing the feasible connectivities is a great challenge due to lack of industrial applications. Therefore, information exchange with practitioners is of high significance. For the construction of the synthesis model, units (feedstocks, processes, intermediates, products) are linked to each other via connections. The “activation” of a connection depends on the formulation of the model. The abovementioned synthesis model is optimized using the GAMS environment and taking into consideration economic data, it results to the optimal paths based on the developed superstructure. For the purpose of this study, a case for the extraction of high-value chemicals from microalga Dunaliella is analyzed as part of the D-Factory, an FP7 collaborative project.

The combination of a superstructure design and an optimization model tackles the designing problem in the field of microalgae biorefineries and offers guidelines for the development of more advanced and detailed design analysis. This methodology acts as a benchmark for a future multicriteria model for the selection of optimal paths regarding the capitalization of microalgae for high-value chemicals.

Process design of 5-hydroxymethlfurfural (5-HMF) Process and integration in bio-refineries

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Replacing crude oil derived chemicals by bio-chemicals is one of the vital actions toward achieving sustainable energy systems. Bio-refineries play an important role for production of bio-fuels and bio-chemicals. 5-hydroxymethylfurfural (5-HMF) is one of the main bio-chemicals that can be produced in bio-refineries as a valuable platform for production of other valuable bio-chemicals.

The goal of this study is to present an assessment on production of 5-HMF from lignocellulosic biomass in an integrated bio-refinery based on the published data in scientific journals. This work studies three different conversion technologies which are named after the reaction environment of the process and are called as biphasic system, ionic liquid system and aqueous phase system. These processes are simulated in Aspen Plus® and evaluation of their energy consumption and economic parameters are presented. Combined heat and power generation is also implemented for further improvements. Result for three studied technologies indicates that biphasic system has the best investment rate of return and annual profit. Ionic liquid system presents a process that is suitable for high capacity productions and in the end, aqueous phase system demands the lowest total investment cost for a profitable plant.

A supply chain optimisation approach to the design of lignocellulose-based products

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Second-generation biorefineries are characterised as complex systems, due to the plethora of processing paths that leads to multiple biobased products, such as biofuels and platform chemicals [1]. However, market uncertainties (e.g. demand and prices) as well as high capital costs hamper the development of such production systems in an economically sustainable manner. Optimisation modelling could help overcome such barriers and also play a central role as a decision-making tool for investing in these technologies [2].

This work aims at the integration of a technology superstructure with a spatially explicit, multi-period, multi-feedstock and multi-echelon, lignocellulosic biomass-to-biobased products supply chain network, formulated as a mixed-integer linear programming (MILP) model The proposed model is solved in GAMS® software platform, using CPLEX solver. The optimisation task of this study is the identification of the profit-based optimal configurations of the overall biorefining network, in a specific geographical context, that satisfy a deterministic biobased market demand over a long-term planning horizon. The decision variables of the model are related to all the entities involved in the examined supply chain, particularly, considering both planning (i.e. cultivation and storage sites, plant size and location) and operational (i.e. logistics and biomass mix) characteristics. A European case study of the South-West of Hungary has been used to demonstrate the applicability of the model, along with its effectiveness in driving decision-making regarding the strategic design of advanced biorefining systems.

The model is populated with selected lignocellulosic feedstocks, conversion paths and biobased products. The performance of sensitivity analyses as well as the inclusion of technical or economic uncertainty metrics into the mathematical framework are of significant importance to the identification of the major cost drivers along with the design and planning of robust biobased supply chains.

Keywords: biobased supply chain optimisation; decision-making; MILP model; technology superstructure

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Development of semantically-enabled community hubs in biorefineries and biorewables

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The production of chemicals and fuels based on biomass has been steadily increased, as a consequence of the environmental issues that have arisen by fossil fuels in addition to the steady decrease of their reserves. Aim is the development of competitive industries based on renewable resources1,2. In order to do this, it is necessary to explore possible chemical products from any possible bio-based feedstock and to optimise the corresponding processes.

There is a huge potential in capitalizing fragmented work around the world, since this would assist and accelerate the progress in both research and industrial communities. The objective of this work is to integrate biomass pathways, models and tools for biorefineries and create a repository that contains information on these existing biomass pathways and models. The challenges that arise here are mainly two. Firstly is the extremely large number of possible pathways and large amount of available data and models that correspond to the pathways. The available information needs to be organised in a systematic way that would also provide easy access to it. The second important challenge is the diversity of the information. The designed tool needs to provide easy management of different types and scales of data (e.g. physical properties, reaction), models (e.g. conceptual, flowsheet) and tools (e.g. ASPEN, gPROMS, MatLab).

An ontology engineering approach will be presented that emulates the types of data as they are available in selected projects, mainly RENESENG3 but also others. The aim is to develop an intelligent environment able to scale-up to also include and organize resources outside the current project. Ontology engineering has recently attracted a lot of attention in chemical engineering community for managing, searching and enriching knowledge4,5. Advantages of ontology engineering include the classification of large amount of information, the classification of complex relations, as well as the generation of new information by the use of reasoners. The services of the repository will include (a) access to all data included in the tool, (b) support for high-throughput search and analysis (c) easy management of available data, (d) synthesis technologies, and (e) uploading of new data of a variety of scales and types from the user. Having a user-friendly interface, the repository targets users of a wide range; from students to engineers in SMEs or international companies. This paper explains the state of progress of the development of the repository for biorefineries and it is presented as a systems call to the academic and industrial community to register their input.

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Rapid capital and operating cost estimation for biorefinery processes under development

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Quick capital and operating cost estimation at the early stages of a process development is crucial for determining the viability of the project and screening the economic potential of alternative routes. Biorefinery processes employ state-of-the-art technologies and thus, represent high risk business decisions. Therefore, preliminary cost estimation during the R&D stages is necessary to help researchers decide wisely on project continuity. Most references rely on literature information to estimate the costs as historical cost data are proprietary information and are seldom announced. They also draw on various costing techniques and heuristics, which were developed for the needs of the petrochemical industry and require high level of process detail, which is not available at the early-stages of the process conception.

We investigated several capital cost estimation methods and reported wide discrepancies in their results, which urge for new developments in the field. The methods rely on "significant process steps" and thermodynamics-based cost estimation relationships and are widely cited in literature, while three well-documented biorefinery processes, are used as validation models. We evaluated the methods' accuracy with means of both deterministic and statistical comparison from reported literature estimates and commercial biorefineries' cost data. As the majority was published during the 1970's-80's and are derived by petrochemical processes, their estimates do not account for the technological progress often met within the state-of-the-art biorefinery processes. Therefore, they are considered obsolete and their use is put into dispute.

We decided to attempt new capital and operating cost estimation methods suitable for biorefineries under development, requiring information available at the start of the process development and within known uncertainty ranges. For the purpose of this work, we have been compiling two databases: the first is composed of cost data from 303 commercial cost biorefinery plants and the second consists of detailed flowsheets from 40 discrete biorefinery processes.

We investigated various process parameters to determine their effect on capital costs. We have developed a new rapid capital cost estimation method, based on curvilinear regression analysis and the "significant process step" approach, which reports the uncertainty around the point estimate. Furthermore, we have developed a new rapid operating cost estimation which requires minimal user input, i.e. the raw materials cost calculation, for determining the net production cost of the process, employing probabilistic means of determination.

Discovering Waste Integrated Valorisation Routes using an Ontology Engineering Approach

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The ever increasing global waste production in combination to the scarcity of materials creates an enormous strain on our resource system [1]. The needs to reduce the use of virgin resources give rise in research areas such as waste Industrial Symbiosis (IS) [2], waste biorefineries, waste valorisation and circular approach economies. Waste resources can considered abundant generated by both industrial and municipal activities. The chemistries or else known as "synthesis paths" to extract materials from waste can also be considered abundant.

Waste is a multicomponent material, containing valuable chemical compounds. If recovered, they can become standalone feedstock or be also integrated with alike feedstocks to be processed by existing industrial facilities. Such sustainable, retrofitting practice will enlarge the process capacity, benefiting from economies of scale, improve LCA performance and cost-effectiveness originating from waste's off-market prices [2].

To achieve such task, a) to appropriately integrate waste resources with virgin feedstocks and b) to identify suitable alternative synthesis paths, producing diverse products, requires the use of two well-established research fields: ontology engineering and mathematical optimisation. Therefore, it is firstly required a large well-structured database to organise knowledge, achieving interoperability of information across various manufacturing organisations and processing facilities. Secondly, an optimisation based decision support platform is necessary to take into consideration all three decision resolution levels: strategic, tactical and operational [3].

This work provides a framework that combines an ontological based platform with an optimisation process systems tool to first organise and manage tacit knowledge such as chemistries, process models, paths, technology specifications, feedstock characteristics etc. for knowledge sharing across cooperative processing units [3] and secondly to discover the optimum synthesis path according to set environmental, economic and technical objectives [4]. The semantic algorithm is used to establish layers of interactions and translate process models into networks that are further fathomed using optimisation and superstructure technology.

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An ontology supported model discovery and data integration

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This paper presents an automated model discovery for the purpose of model and data integration using ontological approach. The proposed approach uses a semantic representation of process system models and data by their input and output streams, as well as descriptions of the functionality. Additionally, the Semantic Web Services (SWS) is employed to create a semantic profile of models and data representing with focus on biorefining processes. To this end, the domain ontology assures unified description of models by guiding the model registration and hence instantiation of ontology through ontology parsing, whereas the SWS assures the process of model discovery, its invocation and consequently integration.

This work is intended to address the challenges that previous research, CAPE-OPEN framework has faced and hence to minimise user intervention in selecting a model for the purpose of model integration. To enable automated discovery process to reduce the reliance of user intervention, the input-output (I/O) matching technique is employed to permit for a high degree of flexibility by allowing a partial matching rather than a full (exact) matching between I/O parameters. In order to demonstrate proposed approach, this methodology is applied to the models in the domain of biorefining, whose inputs and outputs are mainly focused on the key parameters of material streams, as well as functionality characterised by the type of process units with key parameters. The options of the discovered models to the requesting model, in this case model representing fermentation process, is reviewed for its compatibility. The result with an aim to select the best suited model whilst avoiding wrong design solution resulted by inconsistencies of heterogeneous models has been tested.

Techno-Economic Evaluation of Consolidated Bioprocessing of Lignocellulosic Biomass

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The need for environmentally friendly fuels and commodity chemicals has driven research in the production of biofuels and bio derived chemicals, particularly in the production of ethanol. In the biochemical pathway of ethanol production alone, there exists multiple conversion technologies available. One such method, the consolidated bioprocessing proposed by Brethauer and Studer, seems to offer a viable alternative, as high conversion rates are achieved while combining into one reactor the hydrolysis and fermentation steps. [1] This method of using a microbial consortium for conversion would likely open pathways to other liquid fuels and commodity chemicals as well, as similar work has been done in the production of higher carbon alcohols. [2]

However, work has not yet been done to determine feasibility of scale up or to quantify an economic benefit for this method of ethanol production, and that is where this work comes in. Modelling of lab-scale based production allows for technical and economic analysis and optimization, as estimates of energetic efficiency and scale-up potential of novel conversion processes are lacking. Production feasibility will be dependent on the energetic, sustainability, and economic potential of said fuels, especially in comparison to their fossil-fuel derived counterparts. This work presents techno-economic models using flowsheeting software of ethanol production from lignocellulosic feedstock to analyze and compare annual costs and efficiency of the different enzymatic conversion pathways. Furthermore, a method of optimization and comparison of the pathways based on total cost and overall efficiency is then proposed.

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Novelty in reactor design and optimization for biotechnology applications using a systems approach

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Reactors in biotechnology applications are mainly heterogeneous systems that are strongly non-ideal and operate at mild temperatures with several reversible paths in place. Therefore, mass transfer aspects may become crucial as desired products are possible to remove in the course of reaction, eventually improving the overall yields. In contrast with the homogeneous systems, in the heterogeneous schemes, apart from the kinetics and the heat transfer effects, the mass transfer and the general hydrodynamic behavior of the system becomes important. The overall reaction rate depends on kinetics and on the system's ability to exchange mass between different phases. Usually, mass transfer and kinetics are balanced. There is a huge potential for innovation and there is strong evidence that non-conventional reactors are capable to bring significant merits. Still, the design of bioreactors is mainly based on experience and heuristics as they are developed for conventional reactors. Moreover, the diversity of feedstock, along with the complicated activity of the microorganisms used, introduce several design uncertainties to consider.

Significant systems technology is available to cope with multiple paths but a focus on reaction kinetics much less on mass transfer. A systematic approach is proposed in the paper that capitalizes on past knowledge and methods as it is available for multi-phase reactors. The method is intended to support decisions towards unconventional reactors, account for reaction and multi-phase, systems but also consider options for mass transfer aspects and a better link of models with industrial reactors. A superstructure approach has been presented using shadow reactor compartments and following Kokossis & Floudas (1990). The extension of this work will be described considering mass transfer links that are now modeled taking into consideration the implicit arrangement for each shadow compartment (e.g. differentiation between packed bed reactors, fluidized bed reactors, segregated reactors stirred tank bioreactors, tubular bioreactor, airlift bioreactors, etc.). The work capitalizes on the work from a separate community that has provided libraries of correlations that relate mass transfer parameters and holdups with different types of industrial reactors. The methodology uses a superstructure approach that is optimized using evolutionary methods. Results suggest novel sections, novel/non-conventional reactors, and provide for a natural interpretation of optimization results into industrial units. Design parameters include the type of micro and macromixing and the type and size of the industrial reactor. Examples include gas-liquid, solid-liquid, liquid-liquid reaction systems; the methodology could extend for any number of phases.

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Holistic Syntheses of More Sustainable Renewable-Based Supply Networks

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Abstract

The main intention of the companies in the past was mainly focused on the maximization of their economic profit which is clearly understandable because almost no company in the severely competitive market really wants to compromise its profit in order to overcome related environmental and social problems. However, the humanity is significantly changing the ecosystem (Zhao et al., 2005), the world is becoming increasingly resource-constrained (Azapagic & Perdan, 2014), as well as the social dimension is becoming worse. In time of the last big economic recession the rate of the unemployment in the EU (The World Bank, 2016) was increased as well as the inequality in the world in general (Oxfam, 2014). Thus, accurate and effective accounting systems and incentives are needed to map the demand and supply for ecosystem services (Galli et al., 2014) that will also improve the status of society.

This work proposes new sustainability measurements from (multi)national macro-economic and also from a company's micro-economic perspective for the selection of alternatives during multi-objective syntheses of renewable-based supply networks. Economic, environmental and social aspects which form the main three pillars of sustainability are evaluated by a composite monetary term, defined as total profit which is an evolution of the total profit of the past works (Čuček et. al, 2012). Both the burdening and unburdening effects on the environment (Kravanja and Čuček 2013) have been considered. In general in regards to industrial companies (the micro-economic perspective) those incentives are represented by imposed taxes on harmful waste and emissions, as well as by obtained credits for energy conservation, energy efficiency and production of renewable energies in terms of either investments to avoid the burdening or subsidies for producing »green« systems. On the other hand, a macro-economic view is looking at the whole value-chain from the so-called global perspective. A macro-economic view considers the fair prices based on the prevention of the burden associated with the system (Vogtländer et al., 2010), and gives credits for prevention of the burden (Čuček et al., 2012). We propose to include also s-Eco-cost (Delft University of Technology, 2016) which represents social part of sustainable synthesis and consists of compensations to prevent child labour, extreme poverty, reduce fair wage deficit and improve occupational safety and health. Based on those two different views, the differences in obtained solutions in regards to sustainability (economic, environmental and social pillars) are discussed. As unemployment presents one of the most severe problems of the society, number of job positions created will also be considered in total profit.

The presented perspectives are illustrated by two examples: i) heat-integrated biorefinery supply-chain network for the production of second and third generations of biofuels accounting for different biomass sources and different conversion technologies (Čuček et al., 2014), and ii) extended biorefinery supply-chain network by integration of wind and solar, thus forming renewable-based energy supply network (Čuček et al., 2015).

Keywords: Total profit, Eco-profit, Eco-cost, s-Eco-cost, Renewable-based supply networks.

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Optimal management of raceways using meteorological forecasts

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Abstract

Microalgae-based industrial processes are considered a promising technological solution for the production of both high-value compounds and liquid fuels in the transport sector (Chisti (2007)). Focusing on biofuels production, the potential benefits of this technology are not only limited to the high theoretical process productivity related to fast microalge growth rates. In fact, the reduction of the drawbacks associated with first and second generation biofuels and the possibility to couple the production processes with wastewater treatments make microalgae-derived biofuels an important potential substitute for current fossil fuels. Nevertheless, productivity values recorded in large-scale outdoor systems are often sub-optimal and make the current industrial exploitation of this processes economically unsustainable. This drawback is mainly caused by the high complexity of the biological phenomena and the highly fluctuating conditions that occur during the cultivation period, hence the low knowledge of a robust optimal control strategy to be used. Microalgae-based processes require therefore (Bernard (2011)) preliminary efforts on mathematical model building in order to describe in a relative simple way the system dynamics and, consequently, implement a feasible and optimal control strategy. Once a validated model has been found, the task would be reduced to an optimal control problem to maximize a specific metric on a finite time horizon. Light and temperature are the two factors mainly influencing microalgal growth. Average light in the raceway pond is affected by the dilution rate while pond temperature can be controlled by changing the pond depth, and thus the thermal inertia. In this work, we use a biological model (Bernard (2011)) representing the effect of light on photosynthesis and temperature on the overall metabolic activity. This biological model is coupled with a physical temperature model (Béchet et al. (2011)) of the raceway. We use weather forecast data to compute dilution rate and depth which optimize a specific metric of productivity for an open pond system. This approach allowed to achieve a relevant improvement in terms of final productivity with respect to models that do not take into account any temperature effect; moreover, the optimization control strategy has been tested and reduced to a short list of practical and recursive 'rules of thumb' that can be used to simplify future optimization tasks.

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General superstructure synthesis for combined mass and energy optimization in industrial processes

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In the context of fluctuating oil prices and stringent environmental regulations, conservation of energy and curtailing emissions is of significant importance. Process Integration (PI) is a family of methodologies that emerged in response to the oil crisis in 1970s and initially aimed at reducing energy consumption through Heat Integration (HI). It later spread into other fields with the introduction of Mass Integration (MI) or Resource Conservation methods. However, it is important to note that the final goal of these approaches should not be limited to reducing the utility consumption but should also aim to reduce the consumption of raw materials simultaneously. This implies the importance of developing general superstructures for simultaneous mass and energy integration for designing flexible heat and mass exchanger networks. By studying state-of-the-art methodologies, two approaches can be observed: Conceptual vs. mathematical. Conceptual methods tend to be preferred by engineers through using visualisation tools, however they cannot guarantee the optimality of the solution. Mathematical approaches can address global optimality of the solution, however are not easy to use and have convergence issues when dealing with large-size problems, i.e. real industrial cases.

An optimization method based on the Mixed Integer Linear Programming (MILP) has been developed for simultaneous optimization of water and energy (SOWE) in industrial processes. The superstructure integrates process thermal streams and optimizes the consumption of water while maximizing internal heat recovery to reduce thermal utility consumption. To address the complexity of water and energy streams distribution in pulp and paper processes, three features have been incorporated in the proposed SOWE method: **(a)** Non-Isothermal Mixing (NIM) between water streams; **(b)** The concept of restricted matches combined with water tanks has been added to the superstructure; and **(c)** The Integer-Cut Constraint (ICC) technique has been combined with the MILP model to systematically generate a set of optimal solutions to support the decision-making for cost-effective configurations. The improved MILP approach has been evaluated using several examples from the literature. The results indicate that this approach provides in many cases enhanced key performance indicators as compared to the conceptual and nonlinear complex mathematical optimization approaches.

Keywords:

combined mass and energy integration, energy integration, heat exchange network (HEN), multi-criteria optimisation, life cycle assessment, mathematical modelling, superstructure synthesis, uncertainty analysis, wastewater treatment.

Retrofitting of Large-Scale Total Site Heat Exchanger Networks for Fixed and Flexible Designs

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Abstract

Heat and Total Site Integration, and waste heat utilisation can provide considerable energy savings and emission reductions. Currently, energy consumption worldwide is very high and is still growing (BP, 2015). Amongst the sectors, industrial sector consume most of the energy (US EIA 2014) and thus has significant potential for reducing energy consumption. It has been estimated that there are huge potentials for energy savings, such as up to 50 % within the plants (Alfa Laval 2011), and up to 20-25 % of additional energy savings at Total Site level (Hackl et al. 2011). Several approaches have been developed for the purpose of energy savings, such as an approach based on physical insights – Pinch Analysis (PA), an approach based on Mathematical Programming (MP), and combined or hybrid MP/PA and PA/MP approaches. There are two situations regarding energy savings analyses: grassroots for new and retrofit for existing plants and Total Sites. However, considerably more engineering time in the process industries is spent on improving existing production facilities than on designing new plants (Gundersen 2013).

The main focus will be on the developed methodology and procedure by authors for the retrofitting of the existing Total Sites. Methodology and procedure can be applied for plants and Total Sites operating under both steady-state and under dynamic operating conditions. The automated procedure is implemented within software tool TransGen and consists of the three steps: i) Targeting and identification of potential for Heat and Total Site Integration, ii) Identification and selection of retrofitting modifications, iii) Final synthesis of retrofitted Heat Exchanger Network (HEN) (Čuček and Kravanja, 2015). Each step will be presented in detail and demonstrated on illustrative and industrial examples. It will be shown that significant energy savings are possible over a short payback period. Developed methodology and approach might overcome the lack of retrofitting large-scale HENs problems at plant and Total Site levels using MP (Čuček and Kravanja, 2016).

Keywords: Energy savings, Total Site Integration, Heat Exchanger Network, Mathematical Programming, Retrofit

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Climate, Energy, and Food Security from the Sea

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Industrial scale cultivation of marine algae does not require the use of arable land or fresh water and results in biomass yields significantly higher than conventional agriculture. Most research and commercialization efforts have focused on utilizing algae for biofuel production. We show here, through an integrated assessment—using the Global Change Assessment Model (GCAM)—that the co-production of algal fuel and food can lead to significant reductions in greenhouse gas emissions through the offset of agricultural land-use change. Furthermore, production of food products from marine algae can lead to substantial freshwater savings through the direct substitution of water-intensive crops. We compare the strategy of food and fuel co-production to fuel-only and food-only pathways. Generation of fuel is necessary to offset fossil energy inputs and sustain emission reductions. Algal food production, on the other hand, enables food security by increasing production on non-arable land, and significantly reducing land use change. Increasing land availability could enable the development of other low carbon technologies as demonstrated through an observed increase in the production of electricity from terrestrial biomass grown on freed up land. Because algae cultivation requires large amounts of nutrients, development of complementary technologies that deliver recycled nutrients from waste streams will be necessary for large-scale production. If such demands are met, marine algae can enhance food and energy security, while reducing carbon emissions and freeing land for additional emissions reductions strategies.