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Optimal biorefinery product allocation by combining process and economic modeling

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ABSTRACT

The integrated biorefinery has the opportunity to provide a strong, self-dependent, sustainable alternative for the production of bulk and fine chemicals, e.g. polymers, fiber composites and pharmaceuticals as well as energy, liquid fuels and hydrogen. Although most of the fundamental processing steps involved in biorefining are well-known, there is a need for a methodology capable of evaluating the integrated processes in order to identify the optimal set of products and the best route for producing them. The complexity of the product allocation problem for such processing facilities demands a process systems engineering approach utilizing process integration and mathematical optimization techniques to ensure a targeted approach and serve as an interface between simulation work and experimental efforts. The objective of this work is to assist the bioprocessing industries in evaluating the profitability of different possible production routes and product portfolios while maximizing stakeholder value through global optimization of the supply chain. To meet these ends, a mathematical optimization based framework is being developed, which enables the inclusion of profitability measures and other techno-economic metrics along with process insights obtained from experimental as well as modeling and simulation studies.

1. Introduction

Current chemical and energy industries are heavily reliant upon fossil fuels, and these fuels are unsustainable and contribute to economic and political vulnerability (US Department of Energy, 2003). Biomass, a renewable resource, has incredible potential to fulfill the energy and chemical needs of society while minimizing environmental impact and increasing sustainability (Bridgwater, 2003). The process of separating biomass constituents and converting them to high value products is known as biorefining, and the integrated biorefinery provides a unique opportunity for reinvigorating an entire manufacturing sector by creating new product streams (Bridgwater, 2003). Economic and environmental sustainability are achieved through the optimal use of renewable feedstocks, and a need exists for a process systems engineering (PSE) approach to ensure maximum economic and societal benefit through minimizing the usage of raw material and energy resources as well as the cost involved in supply chain operations intrinsic to biorefining. The bioprocessing industries are slowly becoming aware of the benefits of infusing PSE methods to this emerging field. To maximize the applicability of such systematic methods and to integrate experimental and modeling work, a unique partnership has been established consisting of researchers in academia and industry along with government entities, equipment vendors and industry stakeholders to procure the wide range of information necessary such as data needed for process simulation models, information on capacity constraints, financial data, and nonlinear optimization techniques. This information is obtained from a variety of collaborations to be formed and strengthened involving industrial partners, internal academic partners in both chemical engineering and business, and external academic sources. This ensures that the data used in the decision making process is realistic and that the research addresses problems of industrial and regulatory interest. The overall goal

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of the current and future work is to develop a system that will enable decision makers to evaluate different production pathways in biorefining in order to maximize net present value while measuring and minimizing environmental impact. Once this system is able to assist in evaluating the economic and environmental performance of biorefining pathways, these technologies may be constructed as a greenfield project, or retrofitted onto an existing facility.

2. Methodology for integrating modeling and experiments

In biorefining, the large number of possible process configurations and products results in a highly complex process synthesis problem that cannot be solved using simple heuristics or rules of thumb. Business decision as well as policy makers must be able to strategically plan for and react to changes in market prices and environmental regulations by identifying the optimal product distribution and process configuration. Thus, it is necessary to develop a framework which includes environmental metrics, profitability measures, and other techno-economic metrics. Such a framework should enable policy and business decision makers to answer a number of important questions like:

- For a given set of product prices, what should the process configuration be, i.e. what products should be produced in what amounts?
- For a given product portfolio, how can process integration methods be utilized to optimize the production routes leading to the lowest environmental impact?
- What are the discrete product prices that result in switching between different production schemes, i.e. what market developments or legislative strategies are required to make a certain product attractive?
- What are the ramifications of changes in supply chain conditions on the optimal process configuration?

In the following sections, the developed framework for answering these questions is presented along with a discussion of some preliminary results.

The introduction of PSE methods into biorefining research provides a systematic framework capable of seamlessly interfacing results generated in simulation studies as well as experimental work. Such a framework is imperative when attempting to combine knowledge and information from a variety of research areas and disciplines. Fig. 1 illustrates the flow of information throughout this framework in order to evaluate available biorefining technology and study the effects of technological breakthroughs and market fluctuations on the answers to the above questions. The objective of this approach is first to create a library of rigorous simulation models for the processing routes along with a database of corresponding performance metrics. Wherever possible, experimental data is used to validate the performance of the simulation models, and for processes that commercial software packages are incapable of describing adequately, the performance metrics are initially based on experimental results until a satisfactory model has been developed. Existing optimization techniques are then used in order to determine a list of candidate solutions that display maximum economic performance subject to constraints on capacity and material balances, and the final process design is selected among the most profitable allocation schemes with an acceptable level of environmental impact.

Fig. 2 shows a schematic representation of the strategy employed for identification of characteristic performance metrics of the individual subprocesses. The simulation models for each process are developed by extracting knowledge on yield, conversion, and energy usage from empirical as well as experimental data. These models are then used to determine variable cost in terms of necessary labor, maintenance, and utilities, as well as fixed cost to be capitalized over an extended yet finite period of time.

Next, if a given process requires the use of a solvent, molecular design techniques such as group contribution are employed to identify alternative solvents that minimize environmental and safety concerns. The solvent design problem can be solved utilizing either reverse problem formulation or mixed-integer nonlinear programming, but the combination of reverse problem formulation with property clustering have been shown to provide a robust solution (Eljack et al., 2006; Eden et al., 2003; Harper and Gani, 2000).

Process integration techniques are then used to optimize the simulation models. Energy integration involves the use of thermal pinch analysis to design heat exchanger networks, and this is accomplished using commercially available software (El-Halwagi, 1997). Software is also available to perform mass integration, which takes place through the use of tools such as mass pinch diagrams and source-sink mapping (El-Halwagi and Maniousiouthakis, 1989; El-Halwagi, 1997). Process integration is an integral step in the model development as it ensures optimal utilization of biomass and energy resources.

Finally, the optimized models are used to generate data for the economic as well as environmental performance metrics. The estimation of environmental performance is achieved through the use of the US-EPA Waste Reduction (WAR) algorithm (Young and Cabezas, 1999). It should be noted, that only the economic and environmental performance metrics are incorporated in the solution framework described below, thus decoupling the complex models from the decision making process. This approach allows for continuously updating the models as new data becomes available without having to change the selection methodology. Similarly, if new processes are to be included for evaluation, an additional set of metrics are simply added to the solution framework, thus making it robust and flexible.

3. Methodology for biorefinery optimization

The optimization framework, which combines the library of processing routes and corresponding economic performance metrics with a numerical solver, is given in Fig. 3. It should be noted here that the environmental performance is not included as an objective function. Environmental impact is difficult to quantify in terms of profit or net present value unless there were monetary penalty functions applied to the categories of impact, thus making it impractical to include environmental impact in the objective function of gross profit. Multi-objective optimization in which Pareto solution curves are defined will result in environmental impact indicators being minimized (Pistikopoulos et al., 1995). But because maximum shareholder value is attained only with optimal economic performance, these solutions with minimized envi-

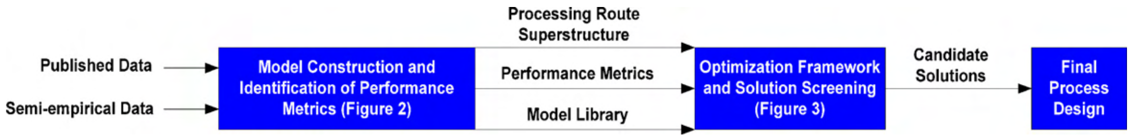

Fig. 1 – Overall data flow.

ronmental impact would not be pursued since the solutions could have an adverse effect on shareholder value in comparison to the economic optimum. One example of this is if optimization were to focus on purely minimizing environmental impact, in which the framework would consequently identify the trivial zero impact facility as a solution, corresponding to no biomass being processed at all and no value being added to the firm or industry in question.

Since multi-objective optimization is impractical without monetizing environmental impact, the objective of the optimization step is to use pre-existing, robust optimization programs to identify candidate solutions that maximize economic performance. The candidates are then ranked according to environmental performance, and thus, environmental performance is used as a screening tool. If a candidate satisfies the environmental objectives, then the optimal production scheme has been identified. If none of the candidates satisfy the environmental impact constraints, then the desired economic performance requirements are relaxed until a solution with acceptable environmental performance has been identified. It should be emphasized that by decoupling the complex models from the optimization and decision making framework, the methodology is more robust and also provides added flexibility by only having to update the performance metrics for a given process as new information, e.g. a new catalyst with higher conversion, is identified. This approach is analogous to the reverse problem formulation framework used for decoupling the complex constitutive equations from the balance and constraint equations of an individual process model (Eden et al., 2004). The design targets linking the two

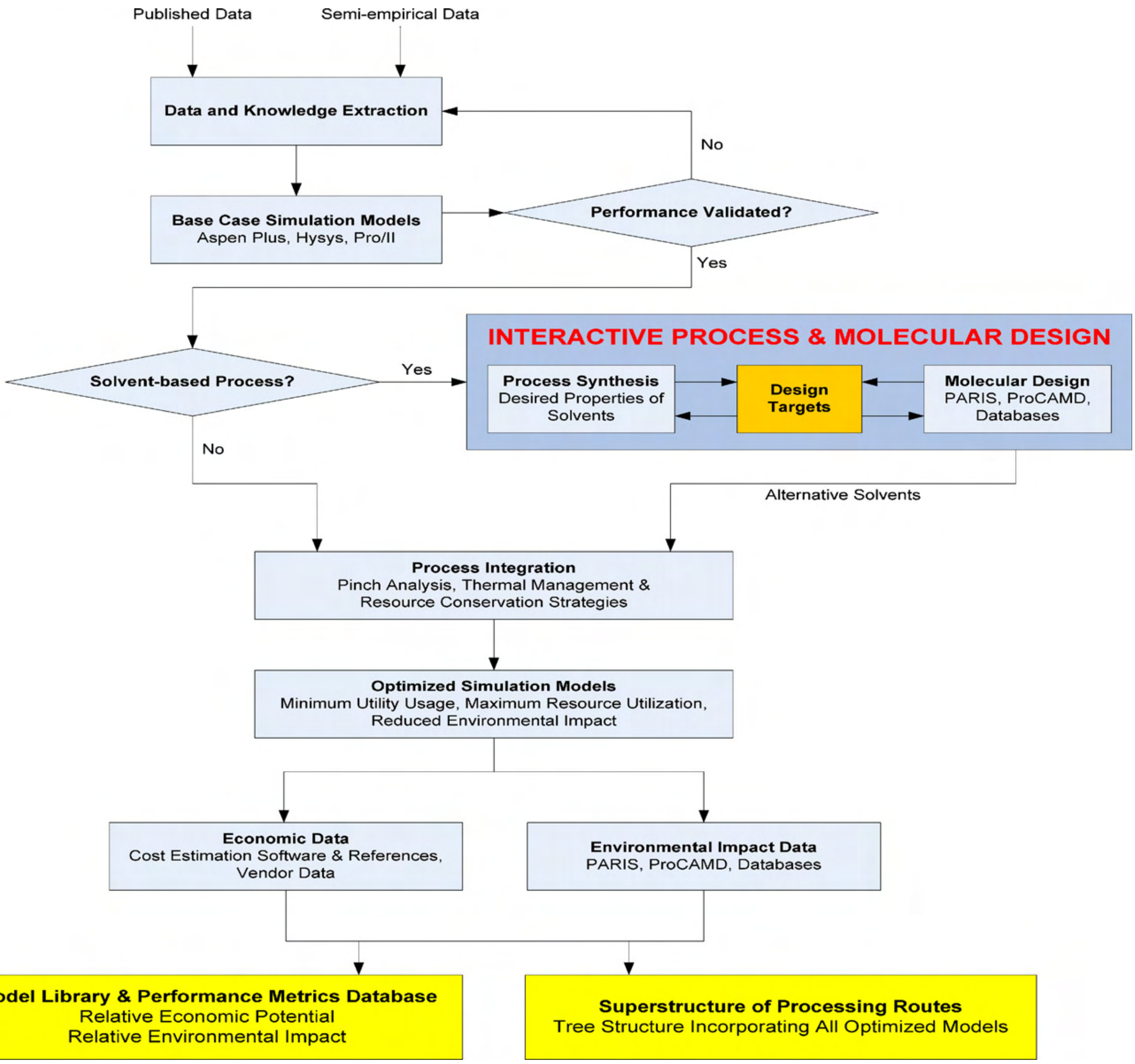

Fig. 2 – Strategy for identification of performance metrics.

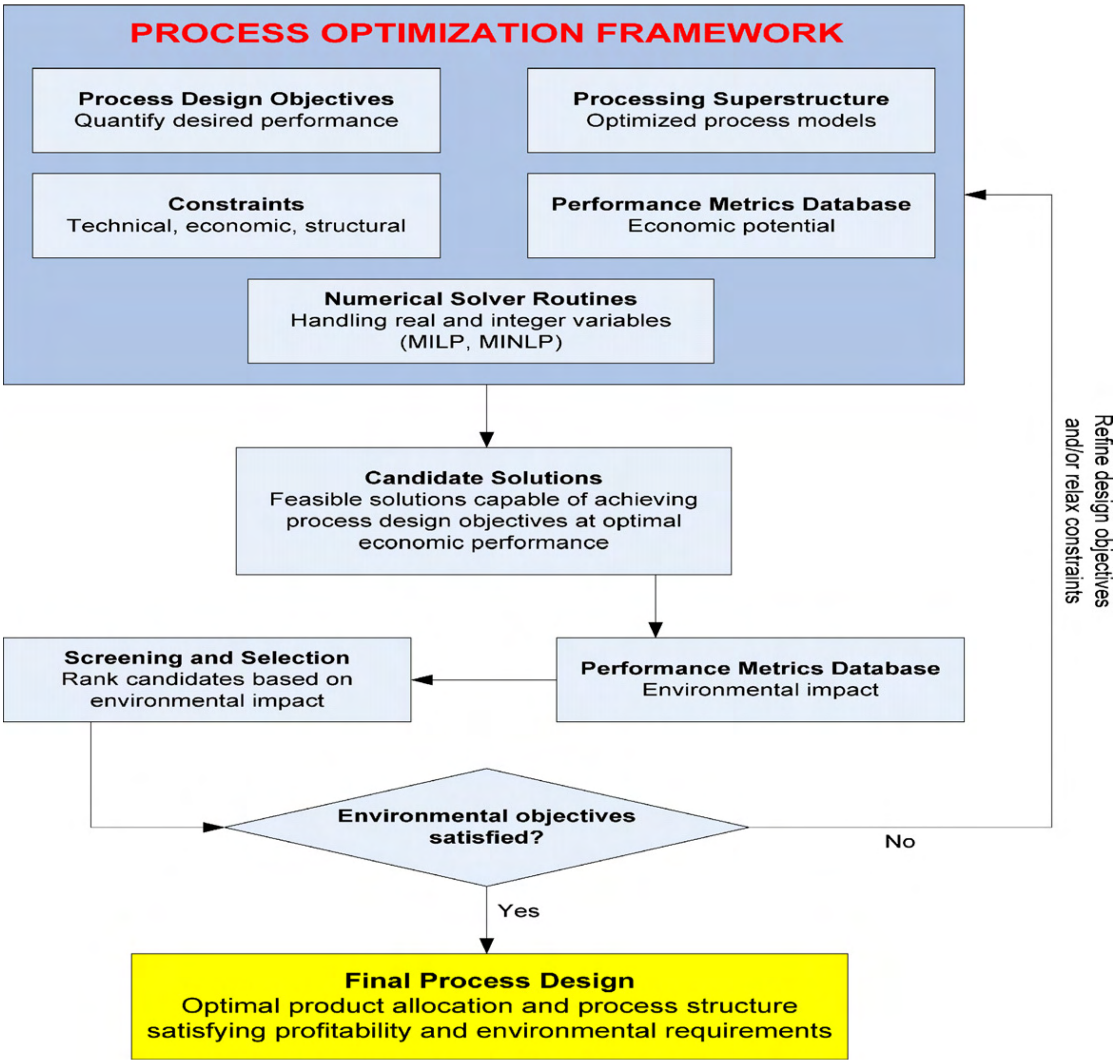

Fig. 3 – Methodology for identification of optimal biorefinery structure.

reverse problems are constitutive or property variables, which in this framework are represented by performance metrics.

4. Scope and complexity of biorefinery production problem

A plethora of combinations of possible products and process configurations exists for the conversion of biomass into chemicals and fuels. Fig. 4 provides an illustration of some of the many processing steps and possible products available in a biorefinery, but it should be noted that it does not include all possibilities and serves primarily to illustrate the complexity of the product allocation problem. The diamonds represent products that can either be sold or further processed to other products, while the boxes denote conversion processes that may be comprised of several processing steps.

It should be noted here that coal is a possible feedstock in the biorefinery illustrated in Fig. 4. Biomass denotes any type of fuel that has an organic source, and this designation ranges from renewable plants and short growth forests to more established non-renewable fuels such as coal and fossil fuels. But because of the recognition of the need to provide energy with minimal environmental impact, the solution may indeed apply to any type of bio-based fuel but would be most helpful in analyzing energy production from renewable feedstocks.

5. Generalized model visualization and optimization

A generalized biorefinery model based on Fig. 4, which has been used to develop the structure of the optimization framework, is given in Fig. 5. The model structure was formulated to include a variety of basic complexities encountered in the decision making process, e.g. whether a certain product should be sold or processed further, or which processing route to pursue if multiple production pathways exist for a given product. The objective function maximizing the overall profit of the biorefinery is given below:

$$\text{Profit}=\sum_{m}\left(\sum_{k}\text{TS}_{mk}C_{k}^{s}-\sum_{i}\sum_{j}R_{mij}C_{mij}^{P}-C_{m}^{BM}\sum_{j}R_{m1j}\right) \quad (1)$$

Using this nomenclature, the first set of terms in Eq. (1) represents the sales revenue from the products made from each

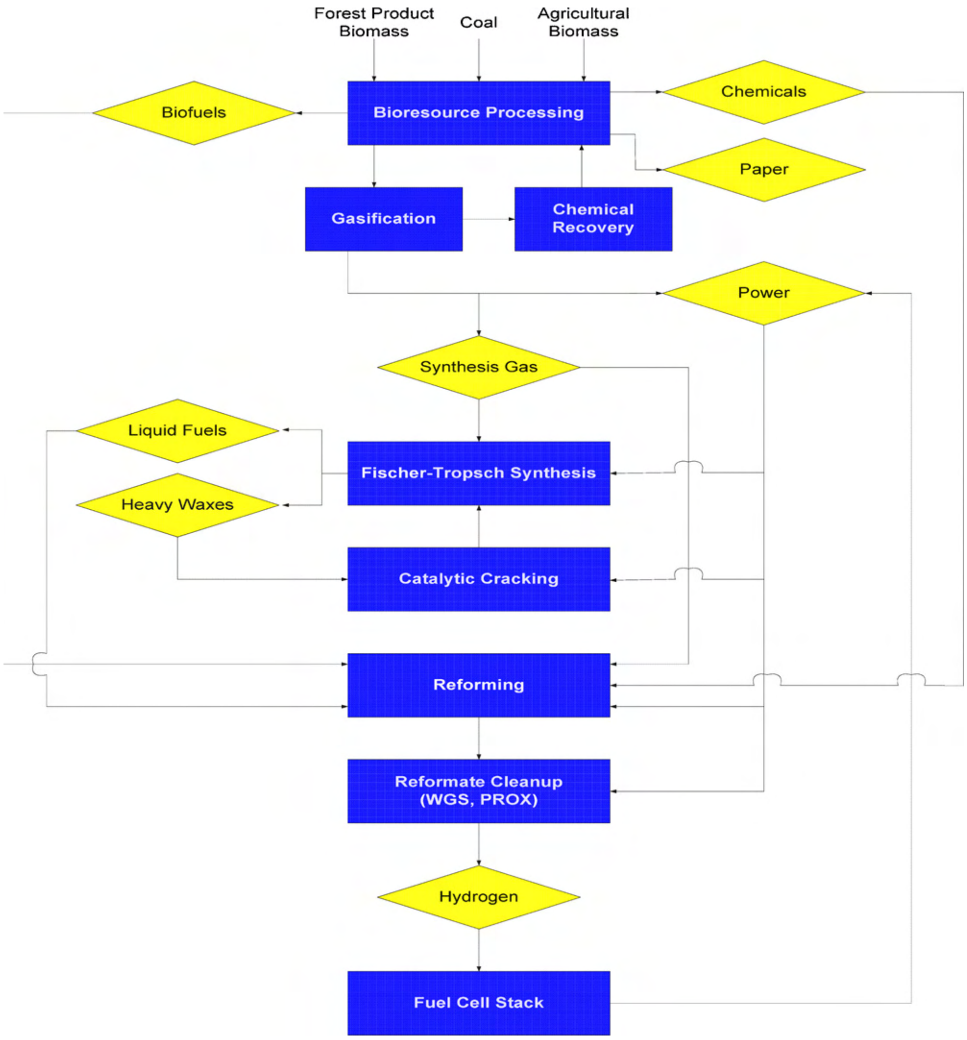

Fig. 4 – Schematic of biomass conversion and biorefinery production rates.

bioresource m. TS_{mk} is a variable that denotes the production rate of product k from bioresource m that is sold to the market. C_k^s is the sales price of product k which is a scalar and is determined through a survey of published prices and vendor quotes. The second set of terms represents the total processing cost incurred by the pathways pursued in production. R_{mij} is a variable that represents the processing rate of route ij while C_{mij}^P is a scalar that represents the cost of processing bioresource m through route ij and is determined through simulation models and process economics. The third set of terms represents the total cost of the biomass resource m, and this is broken down into the scalar pur-

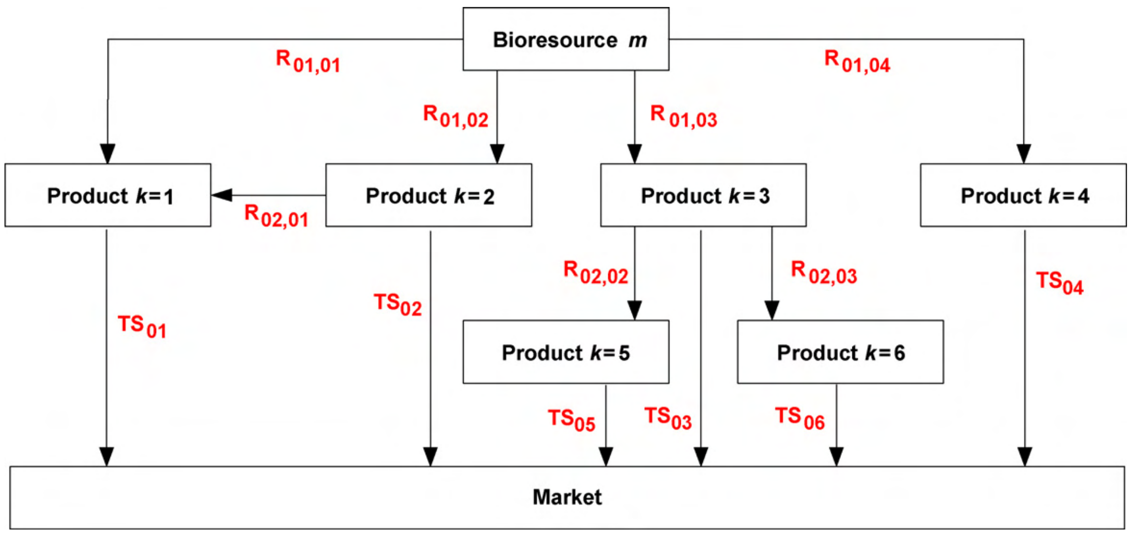

Fig. 5 – Generalized biorefinery model.

chase price of bioresource m in C_m^{BM} and the combined rate of biomass processed by the plant in R_{m1j}. Although both TS_{mk} and R_{mij} are variables in the optimization program, they are not independent since the variables are related to each other via mass balance constraints around the product points. Appendix A shows a detailed list of these mathematical representations.

This generalized model, where the objective function and constraints are linear, is easily solved using commercially available software. It should be noted here that while earlier work such as the proposed solution by Sahinidis et al. (1989) incorporate process models into the optimization problem, the proposed framework separates the wide range of biorefining models from the optimization portion, thus reducing the complexity of the problem for the solver while maintaining the robustness achieved with proven optimization techniques.

Without including any constraints on capacity of the processing steps, the solution is a single-product configuration in which all available biomass is converted into the most profitable product. However, if constraints are imposed on the most profitable route, the framework identifies the additional products and processing routes required to maximize the overall profit, thus leading to a polygeneration facility (Sahinidis et al., 1989). Approximate capacity constraints are based on a variety of sources, e.g. existing equipment, vendor data and qualitative process information provided by academic and industrial collaborators. In order to effectively address the strategic planning objectives of business decision makers, it is necessary to incorporate the total capital investment as a constraint in the formulation. The capital investment for a given unit or process can be approximated as a function of its capacity or processing rate, and both linear and nonlinear expressions have been successfully implemented in the framework. Inclusion of capital cost constraints is crucial for practical application of the results, i.e. enabling evaluation of the potential benefits to be obtained for a given maximum investment by retrofitting an existing facility or constructing new plants.

6. Model demonstration

Many adjustments were made to the parameters such as sales price, processing cost, processing rate conversions, and capital investment functions, and constraints were added on capacity as well as minimum and maximum sales quantities. These modifications were made to determine if the code would give the product distributions that were intuitively determined to maximize profit. In every case, the code returned the solutions including predictable results on the product distribution as well as the pathways necessary to manufacture the product while maximizing value.

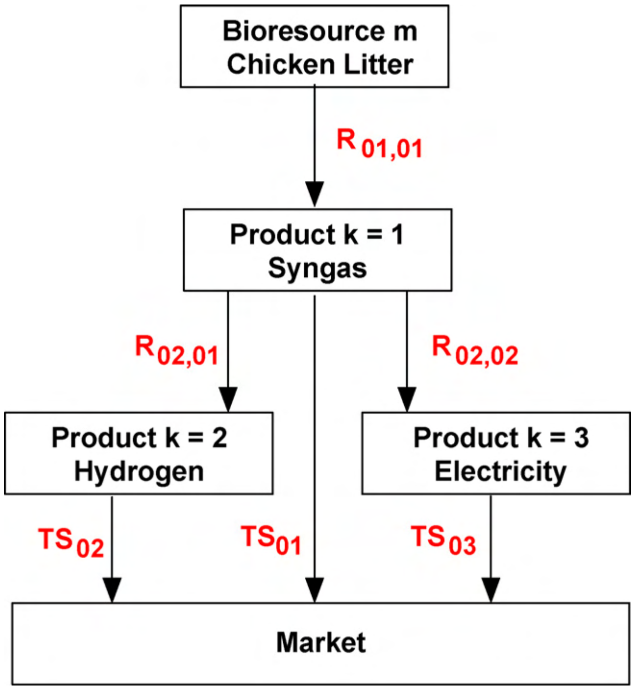

Fig. 6 – Illustration of case study: unsolved decision making tree with variable designations.

To illustrate one particular, simplified example, a case study was performed on a potential biorefinery involving the conversion of chicken litter to syngas, which could be either sold on the market via a pipeline to a local customer, or converted on site into hydrogen or electricity. Conversion into hydrogen takes place through a water gas shift reaction, while electricity is produced through the usage of a combined cycle power island. Base case simulation models were constructed, and data on conversion rates for yields on the gasification, electricity generation, and water gas shift reaction were obtained from literature (Larson et al., 2006; Gadhe and Gupta, 2005). In this example, there are no solvents involved in any of the aforementioned processes, so the step of using property clustering to find safer, more environmentally sound solvents is bypassed. Fig. 6 shows the possible pathways for production and sale of these chemicals on the commodity market, and Figs. 7–9 illustrate the simulation models used in the case study. Due

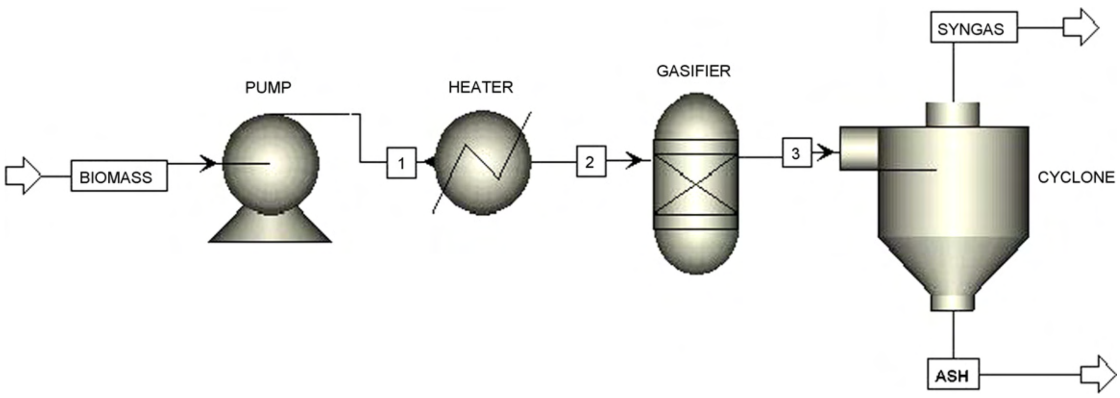

Fig. 7 – Illustration of biomass to syngas simulation model.

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Table 1 – Fixed cost, variable cost, annual output, and cost per output of each simulation model

	Biomass to syngas	Syngas to electricity	Syngas to hydrogen
Total fixed cost	\$112,302,000	\$100,091,000	\$461,527,000
Annualized fixed cost @ 8% interest over 25 years	\$10,401,000	\$9,270,000	\$42,745,000
Total variable costs	\$13,618,000	\$15,301,000	\$202,114,000
Total annual product costs	\$24,019,000	\$24,571,000	\$244,859,000
Annual output	$4.018{*}10^8$ kg	$1.065{*}10^6$ MWe	$8957{*}10^8$ m^3
Cost per output	\$0.0598/kg	\$23.07/MWe	\$0.273/m^3

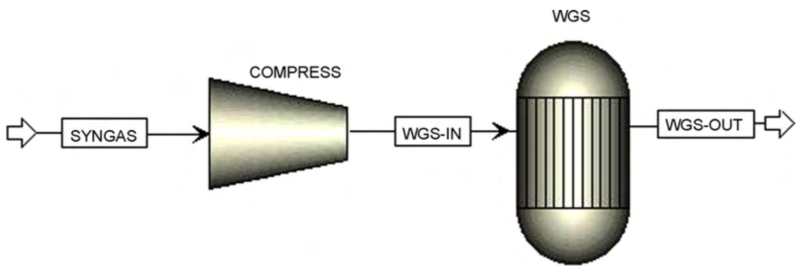

Fig. 8 – Illustration of syngas to hydrogen simulation model.

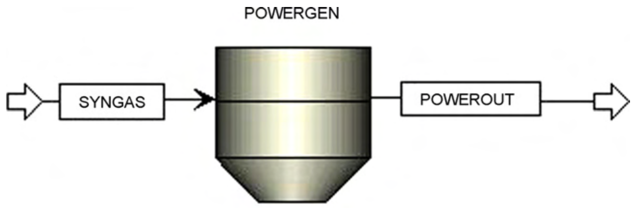

Fig. 9 – Illustration of syngas to power black box model. Details of equipment used in combined-cycle power island are available in Larson et al. (2006).

to the complexity of the combined cycle power island, a black box power generation model is presented for simplicity.

In order to gauge the economic performance of the three processes, it was necessary to procure information on fixed cost, variable cost, and market prices for both feedstock and possible products. The equipment needed for the simulation models was used to determine the fixed cost components of all three processes, and this information is shown in Table 1. Similarly, variable cost was determined using pre-defined design heuristics, and the variable cost is a sum of utilities, operating labor, operating supervision, maintenance, operating supplies, laboratory charges, overhead, and administrative cost as defined by those heuristics (Peters et al., 2003). This component is also included in Table 1. Market prices were obtained through a survey of suppliers, and these prices are listed in Table 2.

Table 2 – Market prices of feedstock and possible products

	Market price
Chicken litter feedstock	\$0.010/kg
Syngas	\$0.214/kg
Electricity	\$53.370/MWe
Hydrogen	\$0.220/m^3

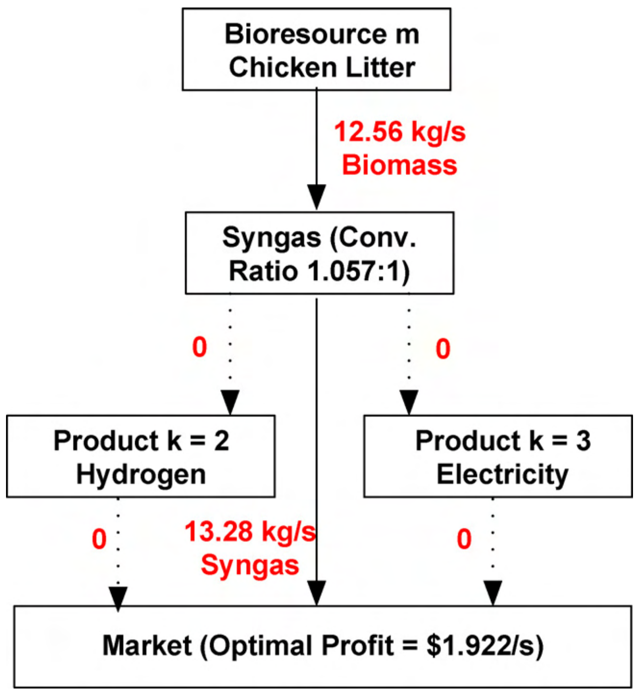

Fig. 10 – Illustration of case study: solved decision making tree with flowrate values and objective function.

In this example, the objective function to be maximized is as shown in Eq. (2)

$$\begin{aligned}\max \text{Profit} = {} & \text{Revenue}_{\text{syngas}} + \text{Revenue}_{\text{hydrogen}} \\ & + \text{Revenue}_{\text{electricity}} - \text{Cost}_{\text{syngas}} - \text{Cost}_{\text{hydrogen}} \\ & - \text{Cost}_{\text{electricity}} - \text{Cost}_{\text{feedstock}}\end{aligned} \quad (2)$$

This objective function is subject to constraints based on mass balances of the individual processes in which a multiplicative conversion rate has been determined so that the conversion of feedstock to output of a given process is linear. The optimization program also contains constraints on the amount of feedstock available, so that a pre-determined feed basis will determine how much is produced, which in turn will be related to gross profit through market prices, processing cost, and feedstock cost.

Due to the simplicity of the problem, the optimization was executed in one iteration through the use of CPLEX in 0.035 s and determined the optimal objective value of $1.922/s profit. The execution of the optimization code verified the results obtained from manual calculation; producing syngas from chicken litter and selling it on the market would maximize profit due to the high costs involved in converting the syngas to hydrogen or electricity. Fig. 10 illustrates the active pathway chosen by the optimization program. This simple case study will be expanded to include a much wider range of products, production pathways, and feedstocks in order to become a crucial decision support tool in the emerging field of biorefining.

7. Conclusions and future work

A general systematic framework for optimizing product portfolio and process configuration in integrated biorefineries has been presented. Decoupling the process models from the decision-making framework reduces problem complexity and increases robustness. The next phase of this work involves development of additional process models for the generation of performance metrics, specifically information on conversion, yield, and production cost for economic metrics and data to be used to generate a measure of environmental impact. From there, process integration will be utilized to optimize the process models by reducing energy usage, material consumption, and waste streams.

An alternative formulation of the product allocation problem will be developed using a combination of general disjunctive programming (GDP) with the use of genetic algorithms (GA) as proposed by Odjo et al. The current formulation of the problem is a mixed-integer nonlinear problem (MINLP), and the use of GA and GDP has been shown to solve non-convex, discontinuous optimization problems more efficiently than the iterative MILP-NLP approach used in many solver programs. The alternative formulation would involve constructing logical disjunctions to map out the decision making tree and decoupling the system of disjunctions from the optimization portion of the framework. The disjunctions will then be converted into "chromosomes" of decision variables, and genetic algorithms will then be used to determine which combination of mixed integers would result in the optimal solution. At this point, the computation time and objective values of optimal solutions between the two solution methods will be compared to determine which formulation is more effective in solving this general problem (Odjo et al., 2008).

The framework will also become a stronger financial tool through the incorporation of various economic ideas and analyses. The use of net present value as a profitability measure in a similar fashion to Sahinidis et al. (1989) will enable the inclusion of the cost of capital, interest expenses, depreciation, and tax consequences of pursued decisions. The development of qualitative predictive models for capital investment and inclusion of capital amortization into the objective function will also increase the strength of the framework. Incorporation of options theory into the framework will allow management to develop financial strategies in response to events in the market or legislative environment. Finally, optimization under uncertainty will be studied to quantify the effects on process configuration resulting from minute changes in product prices (Banerjee and Ierapetritou, 2003). This, in combination with implementing superstructure generation techniques, will lead to increased robustness of the methodology and thus better recommendations (Chakraborty and Linninger, 2003).

Appendix A. List of mathematical representations

C_k^s	scalar, sales price of product k
C_m^{BM}	scalar, purchase price of bioresource m
C_{mij}^P	scalar, cost of processing material from bioresource m through route ij
i	subscript for processing level, or number of processing steps from raw material, i.e. 1 for direct processing of raw material, 2 for subsequent processing step
j	subscript for pathway at that particular processing level
k	product subscript
m	subscript denoting type of biomass resource
R_{mij}	variable, amount processed in route ij from bioresource m
TS_{mk}	variable, total amount of product k produced from bioresource m to be sold to market, related to R_{mij} through mass balance equations

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