Optimal Biorefinery Resource Utilization by Combining Process and Economic Modeling

N.E. Sammons Jr.,[a] W. Yuan,[a] M.R. Eden,[a] B. Aksoy[b] , H.T. Cullinan[b]

[a]*Department of Chemical Engineering, Auburn University, Auburn, AL 36849*
[b]*Alabama Center for Paper and Bioresource Engineering, Auburn University, Auburn, AL 36849*

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.

Keywords: Biorefining, sustainability, optimization, process modeling

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.

2. 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. Figure 1 provides an illustration of some of the many processing steps and possible products available in a biorefinery, but it should be noted that Figure 1 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 is apparent that such a large number of possible process configurations and products results in a highly complex problem that can not 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.

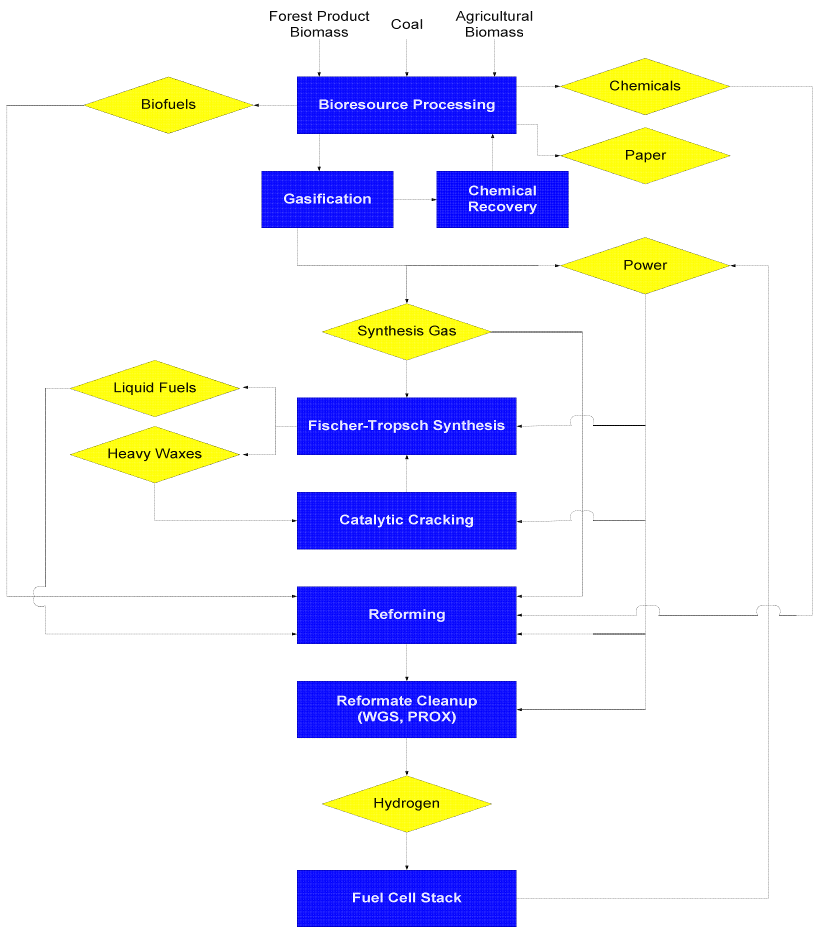

Figure 1 – Schematic of biomass conversion and biorefinery production rates.

3. Methodology for Integrating Modeling and Experiments

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. The objective of this approach is 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.

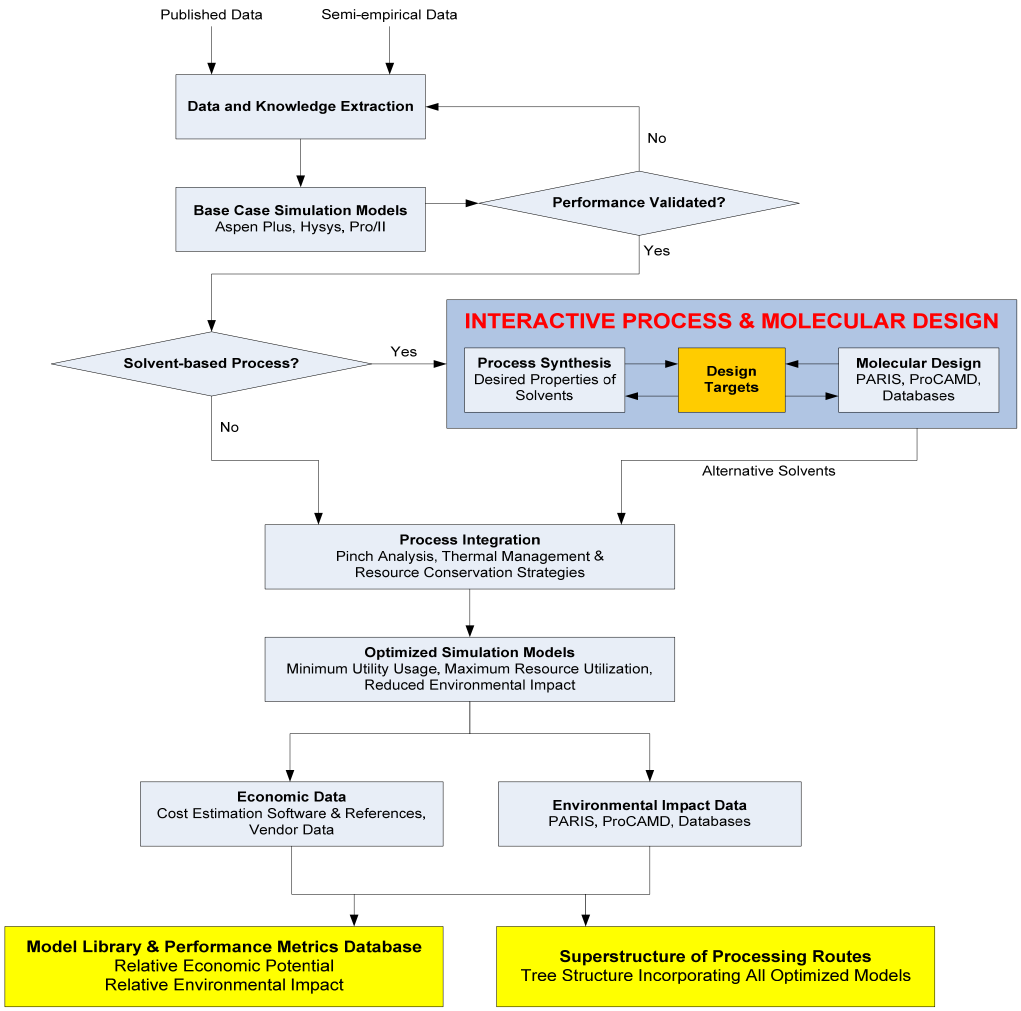

Figure 2 – Strategy for identification of performance metrics.

Figure 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. If a given process requires the use of a solvent, molecular design techniques like CAMD and property clustering techniques are employed to identify alternative solvents that minimize environmental and safety concerns [Eden et al., 2003; Harper & Gani, 2000].

Process integration techniques are then used to optimize the simulation models. This 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 & 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.

4. 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 Figure 3 below. It should be noted that the environmental performance is not included in the optimization step, thus avoiding identification of the zero impact facility as a solution, corresponding to no biomass being processed at all.

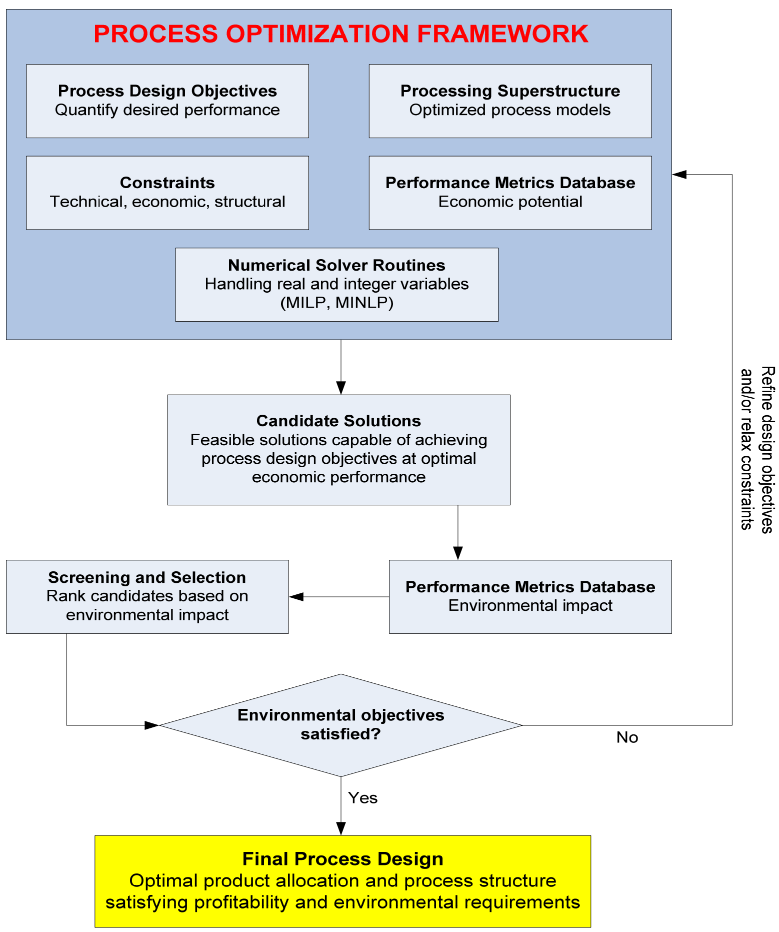

Figure 3 – Methodology for identification of optimal biorefinery structure.

The objective of the optimization step is to identify candidate solutions that maximize economic performance and then the candidates are ranked according to environmental performance. 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 reverse problems are constitutive or property variables, which in this framework are represented by performance metrics.

5. Generalized Biorefinery Model

A generalized biorefinery model, which has been used to develop the structure of the optimization framework, is given in Figure 4. 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:

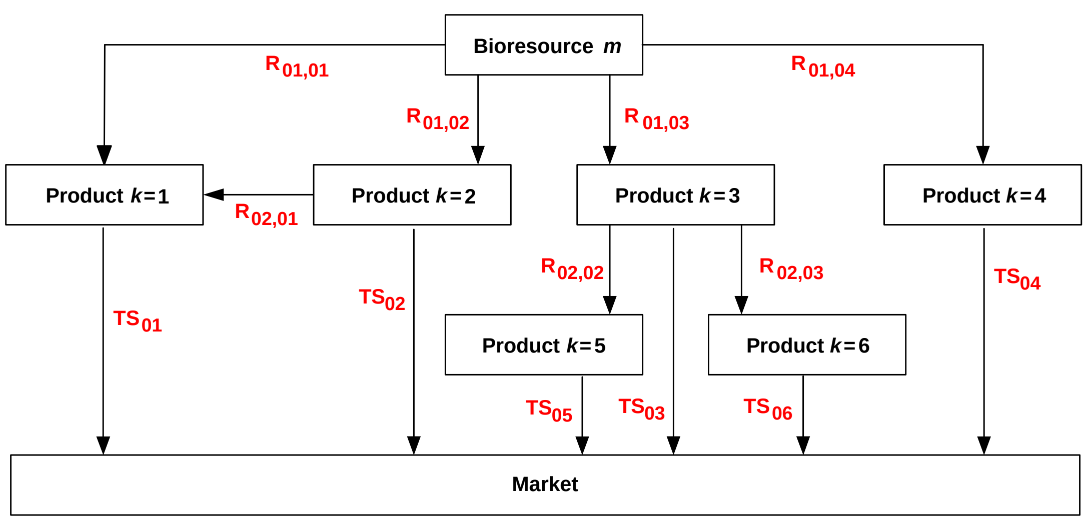

Figure 4 – Generalized Biorefinery Model.

$$\text{Profit} = \sum_m \left(\sum_k TS_{mk} C_k^s - \sum_i \sum_j R_{mij} C_{mij}^P - C_m^{BM} \sum_j R_{m1j} \right) \qquad (1)$$

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

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.

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 Sahnidis and Grossmann [Sahinidis et al., 1989] will enable the inclusion of the cost of capital, interest expenses, deprecication, 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 & Ierapetritou, 2003]. This, in combination with implementing superstucture generation techniques, will lead to increased robustness of the methodology and thus better recommendations [Chakraborty and Linninger, 2003].

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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