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# Fuzzy Optimization Approach for the Synthesis of a Sustainable Integrated Biorefinery

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A shift to utilize more renewable energy sources has been motivated by issues of energy security, environmental protection, and sustainable development. Biofuels are among the promising forms of renewable energy as they can be produced from a wide variety of feedstocks (e.g., traditional agriculture crops, energy crops, forestry products, municipal solid waste, etc.). Biorefineries are processing facilities that convert biomass into value-added products such as biofuels, specialty chemicals, and pharmaceuticals. To enhance material and energy recovery within processing facilities, an integrated biorefinery is proposed. Since the potential pathways and products in an integrated biorefinery are extensive, product allocation is a complex task. The main challenge in designing an integrated biorefinery is to synthesize a sustainable biorefinery with maximum economic performance while causing minimum environmental impact. Since such objectives are often conflicting in nature, fuzzy mathematical programming is adapted in this work to synthesize a sustainable integrated biorefinery that fulfills both considerations simultaneously.

## Introduction

In recent years, the increase of fossil fuel (crude oil) prices, public awareness regarding energy security, sustainable development, depletion of natural resources, as well as environmental concerns, have encouraged the research community to search for sustainable alternative energy sources. Biomass has been identified as one of the potential renewable energy sources to fulfill increasing energy and chemical demands. Biofuels and biochemicals derived from biomass are considered to have inherently lower carbon footprints as compared with equivalents energy derived from fossil fuels. An integrated biorefinery is designed to provide a sustainable supply of biofuels, as well as for the production of bulk and fine biochemicals (e.g., methanol, syngas, glycerol, ether, etc.), with minimum waste generation.<sup>1</sup> Most previous research activities have focused on the improvement of individual biomass conversion platforms.<sup>2</sup> Detailed techno-economic analysis and optimization of well-established biomass-to-energy conversion technologies, such as heat and power generation,<sup>3,4</sup> biodiesel production,<sup>5–9</sup> and bioalcohol<sup>10,11</sup> have been conducted. Currently, there are six commercial scale integrated biorefineries producing mainly ethanol/methanol, power, and heat in the U.S.A.<sup>12</sup> It is noted that less research work has been done on the synthesis of an integrated biorefinery with maximum material and energy recovery systematically. According to Bridgwater,<sup>13</sup> biorefineries will be inherently multifunctional, simultaneously producing biofuels, electricity, and a considerable number of chemicals from biomass inputs via thermal conversion processes. Since both material and energy are recovered within an integrated biorefinery, the overall raw material and energy consumption per unit output are expected

to be lower as compared to conversion processes that operate independently.

As other biomass conversion technologies (e.g., gasification, digestion, Fischer–Tropsch synthesis, etc.) become more established, more alternative processing pathways can be taken into consideration within an integrated biorefinery. Therefore, there is a need to screen all potential pathways systematically and identify potential and feasible pathways that produce the desired products. Recently, Ng et al.<sup>14</sup> proposed a hierarchical approach to the synthesis and analysis of an integrated biorefinery. Two process-screening tools (i.e., Evolutionary Technique and Forward–Reverse Synthesis tree) were presented to analyze and reduce the number of process alternatives in an integrated biorefinery.<sup>14</sup> In addition, Kokossis and Yang<sup>15</sup> identified the challenges of synthesizing and designing sustainable biorefineries, as well as proposed a total systematic approach to combine multiscale formulations with multistage problem solving capabilities for problems involving novel processes. Later, Kokossis and Yang<sup>16</sup> discussed the potential of system tools in the design of complex biorefineries. Most recently, Ng<sup>17</sup> extended the automated targeting approach<sup>18–21</sup> to determine the maximum biofuel production and revenue levels in an integrated biorefinery.

A flexible framework to determine the profitability of different potential production pathways of an integrated biorefinery was developed by Sammons et al.<sup>22</sup> It is noted that only a single objective function (i.e., profitability) problem is considered in the proposed optimization framework. Next, Sammons et al.<sup>23</sup> proposed a general framework for optimizing product portfolio and process configuration in an integrated biorefinery. Sammons et al.<sup>24</sup> then extended their previous work<sup>22</sup> to determine the optimal process pathway based on a more refined economic optimization strategy and environmental performance metrics. In addition, Sammons<sup>25</sup> determined the optimum pathway of an integrated biorefinery with the consideration of both eco-

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nomic and environmental performance via Pareto optimum analysis. However, the previous work is time-consuming as it is iterative in nature. In addition, the unique globally optimal solution may not be generated. Furthermore, Mansoornejad et al.<sup>26</sup> further extend the work in this scope by introducing market aspects, supply chain network design, and flexibility manufacturing design in the framework.

As shown in the previous works,<sup>24,25</sup> multiple optimization objectives are required to be considered in designing an integrated biorefinery. Thus, a fuzzy multiobjective optimization approach is adapted in this work. Fuzzy optimization determines the preferred alternatives in decision making problems by means of solving an objective function on a set of alternatives given by constraints. The preferable alternatives have the more desired (maximum/minimum) objective function values. According to Zadeh,<sup>27</sup> fuzzy systems are especially suitable for the optimization of models that are difficult to derive and contain uncertain parameters. It is noted that this is often the case for reality-based multiobjective optimization problems where the constraints are often estimated. The application of fuzzy theory in optimal decision-making was first presented by Bellman and Zadeh,<sup>28</sup> and it was later extended to linear and nonlinear programming problems with fuzzy constraints and multiple objectives by Zimmermann.<sup>29</sup> The fuzzy multiobjective linear programming approach has been adapted in water network synthesis,<sup>30,31</sup> production planning,<sup>32–35</sup> life cycle analysis,<sup>36,37</sup> retrofit of power sector,<sup>38</sup> energy planning,<sup>39</sup> and Pareto-optimal process configurations.<sup>40–43</sup>

More specifically in the context of integrated biorefinery, Tan et al.<sup>44</sup> adapted a fuzzy multiobjective approach for synthesizing a sustainable energy supply system. An extended input–output model using fuzzy linear programming to determine the optimal capacities of distinct process units based on predefined product demands and environmental goals (carbon, land, and water footprint) was presented.<sup>44</sup>

Although low carbon footprint biomass is used as feedstock, a large-scale biofuel and biochemical production has adverse environmental impact.<sup>44</sup> To synthesize a sustainable integrated biorefinery with maximum economic performance while minimizing environmental impact, a systematic approach to determine the optimum product allocation that fulfills both considerations simultaneously should be developed. Since economic performance and environmental impact considerations are often conflicting in nature, the fuzzy mathematical programming is adapted in this work to determine the optimum integrated biorefinery product allocation based on both considerations. A mixed integer linear programming (MILP) optimization model is presented in this work. Via fuzzy mathematical programming, the inherent conflict between environmental performance and economic considerations can be addressed simultaneously without the need of iteration between environmental objectives and process optimization as found in previous work.<sup>24,25</sup> An industrial case study is solved to illustrate the proposed approach.

## Problem Statement

In this work, the problem definition of an integrated biorefinery can be stated as follows: Given a set of bioresources  $i \in I(B_i^{\text{Bio}})$  with flow rate of  $R_i^I$  can be converted to intermediates  $k \in K$  via technologies/pathways  $j \in J$ . The intermediates  $k$  with flow rate of  $R_k^I$  can be further converted to products  $k' \in K'$  via technologies/pathways  $j' \in J'$ . The conversion of bioresources  $i$  to intermediates  $k$  ( $V_{ij}^I$ ) and intermediates  $k$  to products  $k'$  ( $V_{kj'}^I$ ) via technologies/pathways  $j$  and  $j'$ , respectively, are

also specified. The total production rate of intermediates  $k$  and products  $k'$  are given as  $T_k^{\text{Inter}}$  and  $T_{k'}^{\text{Prod}}$ , respectively. Other than producing intermediates  $k$  and products  $k'$ , technologies/pathways  $j$  and  $j'$  also generate energy (i.e., steam and electricity) via material and energy recovery. The production of energy  $e \in E$  per unit of bioresources  $i$  or intermediates  $k$  via technologies/pathways  $j$  or  $j'$  are specified as  $V_{ije}^{\text{Energy I}}$  and  $V_{k'je}^{\text{Energy II}}$ , respectively. The total production rates of energy  $e$  are given as  $T_e^{\text{Energy}}$ .

The potential environmental impact (PEI) of each pathway  $j$  ( $\text{PEI}_{ijk}^I$ ) and  $j'$  ( $\text{PEI}_{k'k'}^I$ ), which is determined based on the emission, chemical species, and utilities consumption, is also specified in this work. In addition, potential environmental impact of bioresource  $i$  ( $\text{PEI}_i^{\text{Bio}}$ ), final product  $k'$  ( $\text{PEI}_{k'}^{\text{Prod}}$ ), and energy  $e$  ( $\text{PEI}_e^{\text{Energy}}$ ) are included to determine the total potential environmental impact ( $\text{IMP}^{\text{Total}}$ ) of the synthesized sustainable integrated biorefinery. Note that PEI represents the general environmental performance of each individual chemical, processing pathway, etc., which is calculated based per unit of bioresources, final products, energy, and pathways. Therefore, any sustainable matrix and measurement (e.g., global warming potential, aquatic toxicity potential, life cycle analysis, etc.), which normalized based on a same basis can be adapted in the proposed model. In this work, Waste Reduction (WAR) algorithm, which presented by U.S. Environmental Protection Agency is utilized to evaluate the sustainability of the synthesized process.<sup>45</sup>

In addition, the cost of each bioresource  $i$  ( $C_i^{\text{Bio}}$ ), processing cost via technologies/pathways  $j$  ( $C_{ijk}^I$ ), and  $j'$  ( $C_{k'k'}^I$ ), as well as revenue of each product  $k'$  ( $C_{k'}^{\text{Prod}}$ ) are also specified to determine the overall economic performance of the synthesized biorefinery. As shown previously, energy (e.g., steam, electricity, etc.) can be generated from technology/pathways  $j$  and  $j'$ . Thus, to enhance the economic performance of an integrated biorefinery, the generated energy can be exported at the price of  $C_e^{\text{Energy}}$ . However, to synthesize a sustainable integrated biorefinery, consumption of energy within the biorefinery should be self-sustained before considering exporting the energy sources. In this work, it is assumed that all energy produced is prioritized for self-consumption.

In this work, the objective is to synthesize a sustainable integrated biorefinery with maximum economic performance and minimum environmental impact via a fuzzy optimization approach. Note that these two objectives will often be conflicting with each other. Thus, to trade off between two optimization objectives, a degree of satisfaction ( $\lambda$ ) for both objectives is introduced. Each flexible target (economic performance, EP, and total potential environmental impact,  $\text{IMP}^{\text{Total}}$ ) has predefined fuzzy goals for its performance, given by a linear membership function bounded by upper ( $\text{EP}^{\text{U}}$  and  $\text{IMP}^{\text{Total,U}}$ ) and lower limits ( $\text{EP}^{\text{L}}$  and  $\text{IMP}^{\text{Total,L}}$ ) as shown in Figure 1. As shown in Figure 1a,  $\lambda$  approaches 1 as EP approaches the upper limit; while  $\lambda$  approaches 0 as EP approaches the lower limit. However,  $\lambda$  has reverse behavior for  $\text{IMP}^{\text{Total}}$  (see Figure 1b), where  $\lambda$  approaches 1 as  $\text{IMP}^{\text{Total}}$  approaches the lower limit and vice versa. To maximize the satisfaction of both objectives, the optimization objective is set as

$$\text{maximize } \lambda \quad (1)$$

In this work, a mixed integral linear programming (MILP) model is presented to synthesize a biorefinery that achieves the

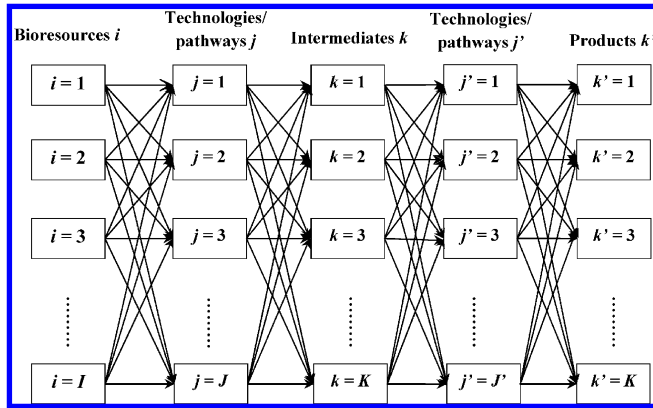


Figure 1. Superstructure for an integrated biorefinery.

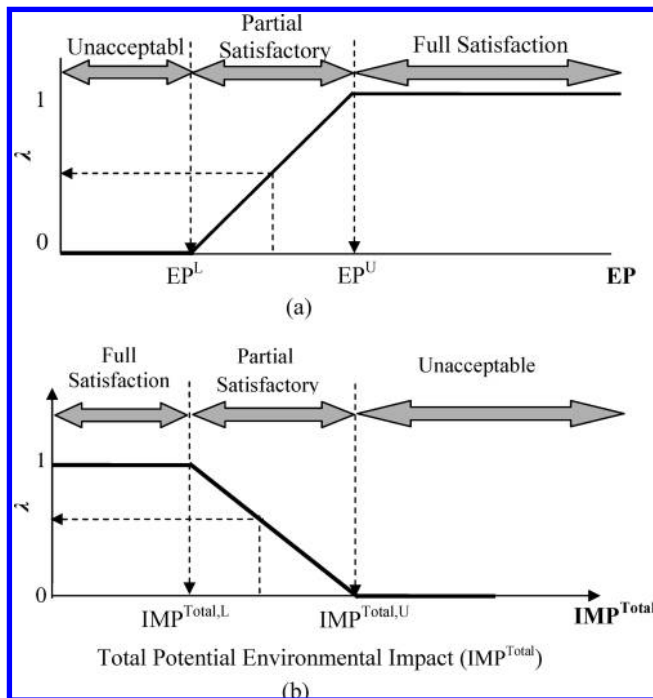


Figure 2. Fuzzy degree of satisfaction ( $\lambda$ ) of the inequalities: (a) economic performance (EP); (b) total potential environmental impact ( $IMP^{Total}$ ).

proposed objectives. The detailed description of the proposed model is presented in the following section.

### Optimization Model

Figure 2 shows a superstructure for the allocation of biore-sources  $i$  to technology/pathways  $j$  to produce intermediates  $k$ , and intermediates  $k$  are further converted to products  $k'$  via technologies/pathways  $j'$  within an integrated biorefinery. Since the detailed allocations of materials and products are essential when synthesizing an integrated biorefinery, the mass flows of biore-sources ( $R_{ij}^I$ ), intermediates ( $R_{kj'}^I$ ), and products ( $T_k^{Prod}$ ) are included in the optimization model. Equations 2 and 3 shows the splitting constraint for biore-sources  $i$  to all potential technologies/pathways  $j$ .

$$R_{ij}^I \leq B_i^{Bio} I_j^I \quad (2)$$

$$B_i^{Bio} = \sum_j R_{ij}^I \quad \forall i \quad (3)$$

where  $I_j^I$  is the binary integer that represents the absence ( $I_j^I = 0$ ) or presence ( $I_j^I = 1$ ) of technologies/pathways  $j$ .

To simplify the network configuration of an integrated biorefinery, the maximum number of potential technologies/pathways  $j$  ( $N_j^{I, \max}$ ) can be specified as

$$\sum_j I_j^I \leq N_j^{I, \max} \quad (4)$$

In addition,  $N_j^{I, \max}$  can also be determined based on various restrictions such as total carbon footprint, amount of biore-sources available, etc.

Biore-source  $i$ , processed in technology/pathway  $j$ , is converted to intermediates  $k$  at the production rate of  $T_k^{Inter}$  with the conversion rate of  $V_{ijk}^I$ . The total production of intermediates  $k$  is given as

$$T_k^{Inter} = \sum_j \sum_i (R_{ij}^I V_{ijk}^I) \quad \forall k \quad (5)$$

Subsequently, the intermediates  $k$  are then distributed to all potential technologies/pathways  $j'$  for further processing to produce the products  $k'$ . The splitting constraint of intermediates  $k$  is given as

$$R_{kj'}^I \leq T_k^{Inter} I_{j'}^I \quad (6)$$

$$T_k^{Inter} = \sum_{j'} (R_{kj'}^I I_{j'}^I) \quad \forall k \quad (7)$$

where  $I_{j'}^I$  is the binary integer that represents the absence ( $I_{j'}^I = 0$ ) or presence ( $I_{j'}^I = 1$ ) of technologies/pathways  $j'$ . Similarly to  $N_j^{I, \max}$ , the maximum number of potential technologies/pathways  $j'$  ( $N_{j'}^{I, \max}$ ) is also specified.

$$\sum_{j'} I_{j'}^I \leq N_{j'}^{I, \max} \quad (8)$$

The total production of product  $k'$  ( $T_k^{Prod}$ ) can be determined via eq 9

$$T_k^{Prod} = \sum_{j'} \sum_k (R_{kj'}^I V_{kj'e}^I) \quad \forall k' \quad (9)$$

It is noted that only two levels of technology/pathway  $j$  and  $j'$  are taken into consideration in this work, as with increasing processing levels, the overall conversion of biore-source to product decreases. In addition, the overall capital investment of the integrated biorefinery will be higher as more process equipments are needed.

In the situation, where a single or no technology/pathway is required to produce the desired final products  $k$ , the biore-sources  $i$  and intermediates  $k$  are allowed to bypass technologies/pathways  $j$  or  $j'$  via a “blank” technology/pathway that does not convert the biore-sources/intermediates.

Via in-plant material and energy recovery, energy can be generated from technologies/pathways  $j$  or  $j'$ . Based on the basis of the given energy conversion of  $V_{ije}^{Energy I}$  and  $V_{kj'e}^{Energy II}$ , the total production of energy streams ( $T_e^{Energy}$ ) from each technology/pathway  $j$  and  $j'$  can be determined by the following equation

$$T_e^{Energy} = \sum_j \sum_i (R_{ij}^I V_{ije}^{Energy I}) + \sum_{j'} \sum_k (R_{kj'}^I V_{kj'e}^{Energy II}) \quad (10)$$

As mentioned previously, to be considered as sustainable integrated biorefinery, the self-consumption of energy requirement ( $T_e^{self-consumption}$ ) should be fulfilled before considering any export. Thus, eq 11 is included in the model.



$$T_e^{\text{Energy}} = T_e^{\text{Self-consumption}} + T_e^{\text{Excess}} \quad (11)$$

where  $T_e^{\text{Excess}}$  refers to the excess energy that can be sold to the grid (for electricity) or to any third party plants at price  $C_e^{\text{Energy}}$ . Note that  $T_e^{\text{Excess}}$  is allowed to be a negative value to indicate inflow/purchase of external energy to the synthesized integrated biorefinery (i.e., when  $T_e^{\text{Self-consumption}} > T_e^{\text{Energy}}$ ).

In this work, the fuzzy multiobjective optimization approach is further extended to synthesize an integrated biorefinery with maximum economic performance while causing minimum environmental impact. To determine the economic performance (EP) of an integrated biorefinery, the overall gross profit per unit time (GP) is utilized in this work and determined via eq 12.

$$\text{GP} = \sum_{k'} T_{k'}^{\text{Prod}} C_{k'}^{\text{Prod}} + \sum_e T_e^{\text{Excess}} C_e^{\text{Energy}} - \left( \sum_i B_i^{\text{Bio}} C_i^{\text{Bio}} + \sum_j \sum_i R_{ij}^{\text{I}} V_{ijk}^{\text{I}} C_{ijk}^{\text{I}} + \sum_k \sum_{j'} R_{kj'}^{\text{II}} V_{kj'k}^{\text{II}} C_{kj'k}^{\text{II}} \right) \quad (12)$$

It is noted that both fixed and variable costs per primary product production rate are taken into consideration in the processing cost of technologies/pathways  $j$  ( $C_{ijk}^{\text{I}}$ ) and  $j'$  ( $C_{kj'k}^{\text{II}}$ ). To determine the net present value (NPV) of the biorefinery's profit/loss over its operational lifespan, eq 13, is included in the model.<sup>25</sup> Note that NPV is a more robust indicator for economic evaluation than using only gross profit. This is because there are many important factors that can be considered in NPV, such as tax breaks from depreciation, incentives or penalties from government as well as hedging cost. In addition, the time value of money should also be taken into account as it is crucial when evaluating profitability of process alternatives.

$$\text{NPV} = \sum_t^{\text{max}} \frac{[\text{GP} \times A(1 - \text{TAX}) + \text{DEP} \times \text{TAX} - \text{HEDGE} + \text{GOV}]}{(1 + R)^t} \quad (13)$$

where  $A$  is the total annual production time for the integrated biorefinery based on the unit time basis in GP. TAX, DEP, and HEDGE are the marginal tax rate, depreciation, and expenses associated with hedging against catastrophic market actions, respectively. GOV and  $R$  are the net benefits realized through government incentives or penalties and expected rate of return or cost of capital respectively; while  $t^{\text{max}}$  is referred as designed lifespan of the biorefinery in term of years. It is worth mentioning that other economic analysis tools such as internal rate of return (IRR), breakeven analysis, etc., can be included in the proposed model for detail economic analysis. For example, NPV in eq 13 can be set as zero to determine the  $R$  when internal rate of return (IRR) analysis is to be performed.

With increasing awareness toward environmental sustainability and stringent discharge limits, many process designers have taken environmental impact as one of the critical parameters in addition to economic metrics when designing a process. Since all processes (e.g., emissions, utilities consumption, etc.), raw materials, primary products, side products, and utilities pose a potential environmental impact (PEI), to determine the relative environmental impact of each chemical species, utilities and processes, a normalized PEI score is to be assigned.<sup>25</sup> In this work, total potential environmental impact ( $\text{IMP}^{\text{Total}}$ ) of a synthesized integrated biorefinery is determined via eq 14. Note that the more negative value of  $\text{IMP}^{\text{Total}}$  represents the synthesized biorefinery is more environmental friendly with reference to the datum score of zero ( $\text{IMP}^{\text{Total}} = 0$ ) when no plant is built.

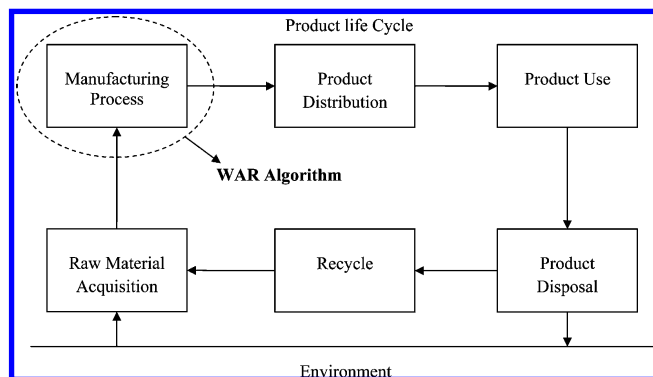


Figure 3. EPA WAR algorithm in relation to overall life cycle analysis.<sup>46</sup>

Note that the negativity in  $\text{IMP}^{\text{Total}}$  score can be obtained by elimination of existing waste streams by sending it for treatment or further processing, instead of discharging it into the environment. Note also that the exported energy contributes positive impact to the total environmental impact score (lower  $\text{IMP}^{\text{Total}}$  score) as exported energy can reduce the amount of energy to be generated by third party. Import of energy to accommodate self-consuming energy within the synthesized integrated biorefinery (i.e., negative  $T_e^{\text{Excess}}$ ) will have a negative effect on the total environmental impact score (higher  $\text{IMP}^{\text{Total}}$  score).

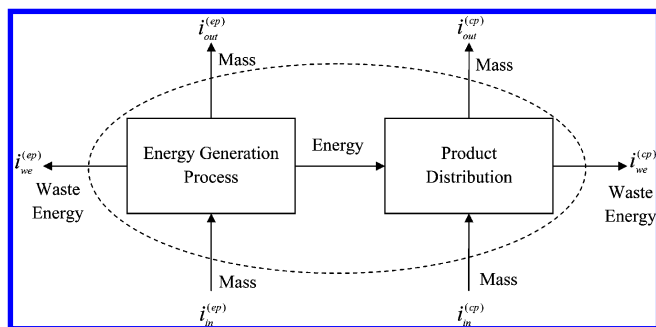
$$\text{IMP}^{\text{Total}} = \sum_{k'} T_{k'}^{\text{Prod}} \text{PEI}_{k'}^{\text{Prod}} + \sum_i \sum_j T_k^{\text{Inter}} \text{PEI}_{ijk}^{\text{I}} + \sum_k \sum_{j'} T_{k'}^{\text{Prod}} \text{PEI}_{kj'k}^{\text{II}} - \sum_e T_e^{\text{Excess}} \text{PEI}_e^{\text{Energy}} - \sum_i B_i^{\text{Bio}} \text{PEI}_i^{\text{Bio}} \quad (14)$$

As mentioned previously, there are various approaches that can be used to measure potential environmental impact. Thus, eq 14 can be modified based on the measurement. In this work, the widely used Waste Reduction (WAR) algorithm proposed by US-EPA<sup>45</sup> is selected as the measurement of sustainability. The WAR algorithm is considered as a subset to overall life cycle analysis (LCA). Figure 3 shows the overall phases of a product's life cycle with consideration raw material acquisition, converting raw material to useful products, distribution and utilization of the products. As shown, the system boundary of the WAR algorithm is focused on the manufacturing process.<sup>46</sup> According to Young and Cabezas,<sup>46</sup> the PEI in the WAR algorithm is defined as the average possible effect based on emissions of mass and energy from a chemical process to the environment. Initially, environmental impact is only measured in term of mass as presented in the following equation:<sup>47</sup>

$$\frac{dI_{\text{system}}}{dt} = i_{\text{in}} - i_{\text{out}} + i_{\text{gen}} \quad (15)$$

where  $dI_{\text{system}}/dt$  is the change in system environmental impact over time,  $i_{\text{in}}$  and  $i_{\text{out}}$  are the input and output rates of impact entering and leaving the process, respectively, and  $i_{\text{gen}}$  is the environmental impact generated within the system.<sup>47</sup> To include impacts from energy generation processes necessary to supply energy to the chemical process, as well as waste energy terms from both the chemical and energy generation processes as shown in Figure 4, eq 15 is modified to

$$\frac{dI_t}{dt} = i_{\text{in}}^{(\text{cp})} + i_{\text{in}}^{(\text{ep})} - i_{\text{out}}^{(\text{cp})} - i_{\text{out}}^{(\text{ep})} - i_{\text{we}}^{(\text{cp})} - i_{\text{we}}^{(\text{ep})} + i_{\text{gen}}^{(\text{t})} \quad (16)$$



**Figure 4.** Impact streams for the chemical and energy generation processes.<sup>46</sup>

where  $dI/dt$  is the accumulation (or depletion) of environmental impact in the given system over time,  $i_{in}^{(cp)}$  and  $i_{out}^{(cp)}$  are the input and output rates of impact in the chemical process,  $i_{in}^{(ep)}$  and  $i_{out}^{(ep)}$  are the input and output rates of impact in the energy generation process,  $i_{we}^{(cp)}$  and  $i_{we}^{(ep)}$  are the impact generated from the release of waste energy to the environment, and  $i_{gen}^{(t)}$  is the impact generated by chemical reactions within the system.<sup>46</sup> As shown in previous works,<sup>46,48</sup> eq 16 can be simplified as

$$i_{gen}^{(t)} = i_{out}^{(cp)} - i_{in}^{(cp)} + i_{out}^{(ep)} \quad (17)$$

where  $i_{out}^{(cp)}$ ,  $i_{in}^{(cp)}$ , and  $i_{out}^{(ep)}$  can be determined via eqs 18–20, respectively.<sup>47</sup>

$$i_{out}^{(cp)} = \sum_a^{cp} M_a^{out} \sum_b x_{b-a} PEI_b \quad (18)$$

$$i_{in}^{(cp)} = \sum_a^{cp} M_a^{in} \sum_b x_{b-a} PEI_b \quad (19)$$

$$i_{out}^{(ep)} = \sum_a^{ep-g} M_a^{out} \sum_b x_{b-a} PEI_b \quad (20)$$

where  $M_a^{out}$  and  $M_a^{in}$  in the above equations represent the mass flow rate of stream  $a$  leaving or entering the process. Meanwhile,  $x_{b-a}$  represents the mass fraction of a given chemical  $b$  in stream  $a$ , and  $PEI_b$  refers the potential environmental impact score of chemical  $b$ .<sup>47</sup> For eq 20,  $ep - g$  represents the gaseous emissions as modern coal-fired power plants can be assumed to be releasing no solid emissions.<sup>47</sup>

The potential environmental impact score of chemical  $b$  ( $PEI_b$ ) can then be determined from the following equation:

$$PEI_b = \sum_l \alpha_l PEI_{b-l} \quad (21)$$

where  $\alpha_l$  is the weighting factor of the impact category  $l$ ,  $PEI_{b-l}$  is the weighted average potential environmental impact score of chemical  $b$  in category  $l$ , which can be obtained from the WAR algorithm software.<sup>48</sup> According to Young et al.<sup>48</sup> the potential environmental impact can be divided into eight main categories, which are human toxicity potential by ingestion (HTPI), human toxicity potential by exposure, both dermal and inhalation (HTPE), terrestrial toxicity potential (TTP), aquatic toxicity potential (ATP), global warming potential (GWP), ozone depletion potential (ODP), photochemical oxidation potential (PCOP), and acidification potential (AP).

In this work, the weighting factor of all eight environmental impact categories ( $\alpha_1 - \alpha_8$ ) are assumed as one that represents all impacts are equally important. Since computation of  $PEI_b$  is

mainly based on types of chemical, such calculation (eqs 15–21) can be removed from the overall optimization model and solved independently.

Fuzzy mathematical programming is adapted in this work, to synthesize an integrated biorefinery with maximum attainable economic performance, while meeting the predefined environmental performance requirement. To allow trading off between both objectives, decision makers are often set an acceptable range for both objectives. In this model, it is assumed that the specified fuzzy goals are having linear membership functions between the upper and lower limits as shown in Figure 1.

A continuous interdependence variable ( $\lambda$ ) is included in the fuzzy model represents the degree of satisfaction for the fuzzy goals. To satisfy the set fuzzy goals of multiple-objectives simultaneously, the optimization objective of  $\lambda$  is to be maximized (as shown in eq 1) subject to the predefined upper and lower limits (eqs 22 and 23) and optimization model (eqs 2–14).

$$\frac{NPV - NPV^L}{NPV^U - NPV^L} \geq \lambda \quad (22)$$

$$\frac{IMP^{Total,U} - IMP^{Total}}{IMP^{Total,U} - IMP^{Total,L}} \geq \lambda \quad (23)$$

where  $NPV^U$  and  $NPV^L$  are the upper and lower limits of predefined NPV,  $IMP^{Total,U}$  and  $IMP^{Total,L}$  are the upper and lower limits of  $IMP^{Total}$ . Since  $\lambda$  is often given as a continuous variable ranged between 0 and 1, eq 24 is also included in the optimization model.

$$0 \leq \lambda \leq 1 \quad (24)$$

The interaction between the two objectives as represented by eqs 22 and 23 indicates that  $IMP^{Total}$  will approach its lower limit, while NPV approaches its higher limit when the maximum degree of satisfaction  $\lambda$  is achieved ( $\lambda$  close to 1). To illustrate the proposed approach, an industrial case study is solved. In this work, a commercial optimization software LINGO, version 10, with Global Solver is used to optimize the proposed mode.

## Case Study

A gasification-based biorefining case study in the kraft pulp and paper industry adapted from Larson et al.<sup>49</sup> is utilized to illustrate the proposed approach. Larson et al.<sup>49</sup> conducted an extensive study on the economic and environmental performances of integrating a hypothetical pulp and paper mill with an integrated biorefinery. In the kraft pulp process, a large amount of lignin-rich byproduct of cellulose fiber, which also known as black liquor (BL), is generated. Currently, energy and pulping chemicals from BL are recovered via Tomlinson recovery boilers.<sup>49</sup> However, as pointed out by Larson et al.,<sup>49</sup> in the next 10–20 years, most of these boilers in the U.S.A. and Europe are approaching their end-of-life and require a high amount of capital investment for replacement.<sup>49,50</sup> Note that the production of liquid fuels and chemicals via gasification of kraft BL and woody residue can generate substantial profits for the industry.<sup>25</sup> Therefore, different alternative pathways for sustainable development, other than replacing existing boiler with new Tomlinson boiler, should be analyzed. Integrated biorefinery, which produces liquid products from BL is identified as one of the most promising sustainable processes. Thus, detailed analysis of energy, environmental impact, and economic cost, as well as the benefits of the BL biorefinery, were conducted.<sup>49</sup> In the

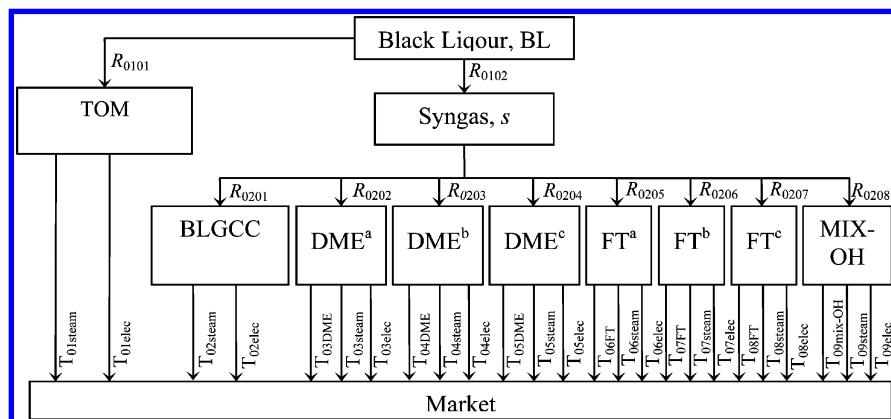


Figure 5. Alternative pathways for black liquor processing.<sup>25,49</sup>

Table 1. Biorefinery Retrofit Options for Existing Pulp and Paper Facilities<sup>49</sup>

process	product range	description
Tomlinson boiler (TOM)	electricity, steam	replacing aging Tomlinson boiler
combined cycle of black liquor gasification (CCBLG)	electricity, steam	replace Tomlinson boiler with combined cycle turbine fired by syngas
dimethyl ether, process a (DME <sup>a</sup> )	electricity (negligible), steam, dimethyl ether	no gas turbine, no wood gasification, 97% recycle of syngas from black liquor gasification through synthesis process
dimethyl ether, process b (DME <sup>b</sup> )	electricity, steam, dimethyl ether	syngas from wood gasification is sent to gas turbine to generate electricity and then steam, 97% recycle of syngas from black liquor gasification through synthesis process
dimethyl ether, process c (DME <sup>c</sup> )	electricity, steam, dimethyl ether	syngas from wood gasification is sent to gas turbine to generate electricity and then steam, one pass synthesis process using syngas from black liquor gasification
Fischer–Tropsch synthesis process a (FT <sup>a</sup> )	electricity, steam, FT liquid	syngas from wood gasification is sent to gas turbine to generate electricity and then steam, one pass synthesis process using syngas from black liquor gasification
Fischer–Tropsch synthesis process b (FT <sup>b</sup> )	electricity, steam, FT liquid	syngas from wood gasification is sent to gas turbine to generate electricity and then steam, one pass synthesis process using syngas from black liquor gasification
Fischer–Tropsch synthesis process c (FT <sup>c</sup> )	electricity, steam, FT liquid	syngas from wood and black liquor gasification is sent to product synthesis, one pass product synthesis process
mixed alcohols synthesis (Mix-OH)	electricity, steam, C1–C3 alcohols	syngas from wood and black liquor gasification sent to product synthesis, 76% recycle of syngas in the synthesis process

previous work,<sup>49</sup> three types of biorefinery liquid products (i.e., Fischer–Tropsch fuel (FT fuel), dimethyl ether (DME) and mixed alcohol fuel) and a combined cycle process are taken into consideration.

Figure 5 shows the potential alternative pathways for BL processing that are proposed by Larson et al.<sup>49</sup> Other than replacing the current aging Tomlinson boiler, various products may be generated from BL. As shown, syngas is first generated from BL gasification via two pressurized, high-temperature gasifiers with oxygen as an oxidant. The generated syngas can then be used in a combined cycle to generate electricity and steam through a gas turbine. Besides, the low pressure syngas (effluent of gas turbine) can be used to produce DME, FT fuel, or mixed alcohol fuel. In this case study, three process configurations of DME production (DME<sup>a</sup>, DME<sup>b</sup>, and DME<sup>c</sup>) from syngas are taken into consideration. In the DME<sup>a</sup> process, DME is produced as the main product, while steam and electricity are generated as side products via a steam turbine. Meanwhile, DME<sup>b</sup> employs an additional biomass gasifier and turbine to produce additional syngas for steam and electricity generation. DME<sup>c</sup> has a similar configuration as DME<sup>b</sup>. The main difference is

that the unconverted syngas is used to generate steam and electricity, instead of being recycled to the DME synthesis reactor in DME<sup>b</sup>.

On the other hand, three different configurations (FT<sup>a</sup>, FT<sup>b</sup>, and FT<sup>c</sup>) of FT fuel production are also included in the analysis. FT<sup>a</sup> produces FT liquids as the main product and generates electricity, as well as steam from unconverted syngas. Besides, additional syngas is generated from biomass via a gas turbine. In FT<sup>b</sup>, a similar process configuration as FT<sup>a</sup> is employed with a different type of gas turbine. In process configuration FT<sup>c</sup>, the generated syngas from biomass gasification is mixed with syngas generated from BL gasification to produce FT liquids. The unconverted syngas is then used to generate steam and electricity via steam turbine. Other than producing DME and FT fuel using syngas, production of mixed-alcohol fuel via a mixed-alcohol process (Mix-OH) from syngas is also taken into consideration. All the above-mentioned process configurations are summarized as Table 1.

It is worth mentioning that all alternatives processes (FT<sup>a</sup>, FT<sup>b</sup>, FT<sup>c</sup>, DME<sup>a</sup>, DME<sup>b</sup>, DME<sup>c</sup>, and Mix-OH) are individually optimized to be energy (e.g., electricity, steam, etc.) self-sustaining.<sup>49</sup> It is assumed that excess energy, which is not

**Table 2. Conversion Factor for Each Technology/Pathway<sup>25,49</sup>**

technology/pathway $ij$	conversion factor $V_{ijk}^I$	intermediates $k$ /products $k'$	value
0101	$V_{0101\text{steam}}$	steam	$5.752 \times 10^{-3}$ (k lb/s steam)/(kg/s BL)
	$V_{0101\text{elec}}$	electricity	$4.537 \times 10^{-4}$ (MWh electricity)/(kg/s BL)
0102	$V_{0102\text{syngas}}$	syngas	1.688 (kg/s syngas)/(kg/s BL)
technology/pathway $kj'$	conversion factor $V_{kjk'}^H$	products $k'$	value
0201	$V_{0201\text{steam}}$	steam	$3.555 \times 10^{-3}$ (k lb/s steam)/(kg/s syngas)
	$V_{0201\text{elec}}$	electricity	$5.274 \times 10^{-4}$ (MWh electricity)/(kg/s syngas)
0202	$V_{0202\text{DME}}$	DME	$3.845 \times 10^{-2}$ (gal/s DME)/(kg/s syngas)
	$V_{0202\text{steam}}$	steam	$3.557 \times 10^{-3}$ (k lb/s steam)/(kg/s syngas)
	$V_{0202\text{elec}}$	electricity	$2.589 \times 10^{-6}$ (MWh electricity)/(kg/s syngas)
0203	$V_{0203\text{DME}}$	DME	$3.845 \times 10^{-2}$ (gal/s DME)/(kg/s syngas)
	$V_{0203\text{steam}}$	steam	$3.557 \times 10^{-3}$ (k lb/s steam)/(kg/s syngas)
	$V_{0203\text{elec}}$	electricity	$4.061 \times 10^{-4}$ (MWh electricity)/(kg/s syngas)
0204	$V_{0204\text{DME}}$	DME	$1.698 \times 10^{-2}$ (gal/s DME)/(kg/s syngas)
	$V_{0204\text{steam}}$	steam	$3.557 \times 10^{-3}$ (k lb/s steam)/(kg/s syngas)
	$V_{0204\text{elec}}$	electricity	$4.185 \times 10^{-4}$ (MWh electricity)/(kg/s syngas)
0205	$V_{0205\text{FT}}$	Fischer–Tropsch fuel (biofuel)	$1.570 \times 10^{-2}$ (gal/s FT fuel)/(kg/s syngas)
	$V_{0205\text{steam}}$	steam	$3.557 \times 10^{-3}$ (k lb/s steam)/(kg/s syngas)
	$V_{0205\text{elec}}$	electricity	$4.053 \times 10^{-4}$ (MWh electricity)/(kg/s syngas)
0206	$V_{0206\text{FT}}$	Fischer–Tropsch fuel (biofuel)	$1.570 \times 10^{-2}$ (gal/s FT fuel)/(kg/s syngas)
	$V_{0206\text{steam}}$	steam	$3.557 \times 10^{-3}$ (k lb/s steam)/(kg/s syngas)
	$V_{0206\text{elec}}$	electricity	$1.058 \times 10^{-3}$ (MWh electricity)/(kg/s syngas)
0207	$V_{0207\text{FT}}$	Fischer–Tropsch fuel (biofuel)	$4.823 \times 10^{-3}$ (gal/s FT fuel)/(kg/s syngas)
	$V_{0207\text{steam}}$	steam	$3.557 \times 10^{-3}$ (k lb/s steam)/(kg/s syngas)
	$V_{0207\text{elec}}$	electricity	$3.573 \times 10^{-4}$ (MWh electricity)/(kg/s syngas)
0208	$V_{0208\text{Mix-OH}}$	mixed alcohol fuel	$9.299 \times 10^{-3}$ (gal/s Mix–OH)/(kg/s syngas)
	$V_{0208\text{steam}}$	steam	$3.557 \times 10^{-3}$ (k lb/s steam)/(kg/s syngas)
	$V_{0208\text{elec}}$	electricity	$4.247 \times 10^{-4}$ (MWh electricity)/(kg/s syngas)

**Table 3. Economic Data for Processing Black Liquor<sup>25,49</sup>**

technology/ pathway $ij$	primary output $k/k'$	fixed and variable cost per primary output $C_{ijk}^I$ (U.S.\$)
0101	steam	4.568/k lb steam
0102	syngas	$5.189 \times 10^{-3}$ /kg syngas
technology/ pathway $kj'$	primary output $k'$	fixed and variable cost per primary output $C_{kjk'}^H$ (U.S.\$)
0201	electricity	39.65/MWh
0202	DME	0.6508/gal DME
0203	DME	1.090/gal DME
0204	DME	1.813/gal DME
0205	Fischer–Tropsch fuel (biofuel)	2.047/gal FT fuel
0206	Fischer–Tropsch fuel (biofuel)	3.445/gal FT fuel
0207	Fischer–Tropsch fuel (biofuel)	1.114/gal FT fuel
0208	mix-alcohol fuel	4.008/gal Mix–OH

utilized in the processes can be exported to the pulp and paper mill. Table 2 shows the conversion factor for each technology/pathway covering intermediates (syngas), products (FT liquid, DME, mixed-alcohol fuels) and energy (i.e., electricity and steam) via technologies/pathways  $ij$  and  $kj'$ .<sup>25,49</sup>

Note that each alternative process contributes to different economic and environment performance.<sup>25,49</sup> Tables 3–5 summarize the economic data and environmental performance measures for all alternative processes. Table 3 shows the total fixed and variable costs (which include annualized capital cost, operating cost, and maintenance cost) per primary main product of each alternative process. For example, the main product of technology/pathway 0202 is DME; thus, the total fixed and variable costs is quoted per gallon of DME produced (see Table 3). It is worth mentioning that all the economic data are extracted from the extensive modeling and rigorous calculations performed by Larson et al.<sup>49</sup> On the other hand, the market price of products and bioresources which was taken from market data

**Table 4. Price of Products and Bioresources<sup>25,49</sup>**

final product $k'$	revenue from final product, $C_k^{\text{Prod}}$ (U.S.\$)
DME	0.99/gal
Fischer–Tropsch fuel	1.54/gal
mixed alcohol	1.77/gal
energy	revenue from energy (US\$)
exported electricity to the pulp and paper mill	$C_{\text{elec mill}}^S$ 56.2/MWh
exported electricity to the grid	$C_{\text{elec grid}}^S$ 40/MWh
steam	$C_{\text{steam}}^S$ 1.534/k lb
bioresources $i$	Cost of raw material (\$)
black liquor	$C_i^{\text{Bio}}$ 0.03223/kg

is showed in Table 4. Note that the product market prices of DME, Fischer–Tropsch fuel and mixed alcohol fuels are the prices in 2005 that Larson et al.<sup>49</sup> used for their detailed economic analysis. As the product prices are listed as independent parameters in the model, it can be revised based on the current market price of each product, together with a costing at present value, for updated economic analysis.

In this case study, it is assumed the total available amount of black liquor,  $B_i^{\text{Bio}}$ , from the Kraft pulp and paper mill is given as 35.6 kg/s. As mentioned previously, all alternative processes are energy self-sustained; thus,  $T_e^{\text{self-consumption}}$  in eq 11 is set as zero ( $T_e^{\text{self-consumption}} = 0$ ). It is assumed that all excess energy,  $T_e^{\text{Excess}}$  (electricity,  $T_{\text{elec}}^{\text{Excess}}$ , and steam,  $T_{\text{steam}}^{\text{Excess}}$ ) will be utilized in the pulp and paper mill ( $T_{\text{elec mill}}^{\text{Excess}}$ ) or sold to the grid ( $T_{\text{elec grid}}^{\text{Excess}}$ ). As shown in previous works,<sup>45</sup> the electricity consumption of the pulp and paper mill is given as  $2.7804 \times 10^{-2}$  MWh/s. The additional electricity generated will then be sold to the grid. However, as shown in Table 4, there is a price difference in electricity utilized in the pulp and paper mill,  $C_{\text{elec mill}}^S$  (\$56.2/



**Table 5. PEI Scores of Emissions for All Processes<sup>25</sup>**

emissions	category of potential environmental impact								PEI score
	HTPI	TTP	HTPE	ATP	GWP	ODP	PCOP	AP	
wood combustion VOC	0.293	0.293	0.027	0.336	0.001	0.000	1.260	0.000	2.210
gas combustion VOC	0.470	0.470	0.265	0.016	0.000	0.000	3.110	0.000	4.330
CO	0.000	0.000	0.004	0.000	0.000	0.000	0.017	0.000	0.021
NO <sub>x</sub>	0.000	0.000	0.009	0.000	0.000	0.000	1.500	1.070	2.580
PM10	3.480	3.480	0.078	0.154	0.000	0.000	0.000	0.000	7.190
total reduced sulfur (TRS)	0.689	0.689	0.007	0.343	0.000	0.000	0.000	0.092	1.820
SO <sub>x</sub> /SO <sub>2</sub>	0.000	0.000	0.018	0.000	0.000	0.000	0.144	0.987	1.150
CO <sub>2</sub>	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
electricity (per MWh)	0.280	0.280	0.004	0.960	0.690	0.000	0.000	21.50	23.70
process steam (per klb)	−0.006	−0.006	0.000	−0.010	0.049	0.000	0.000	0.190	0.217
DME (per gal)	0.046	0.046	0.000	0.000	0.000	0.000	0.625	0.000	0.716
FT (per gal)	0.280	0.280	0.000	0.854	0.003	0.000	2.266	0.000	3.683
MOH (per gal)	0.337	0.337	0.000	0.000	0.000	0.000	1.809	0.000	2.483
black liquor, BL (per kg)	0.470	0.470	0.017	0.002	0.000	0.000	0.000	0.000	0.959
syngas (per kg)	0.000	0.000	0.001	0.047	0.000	0.000	0.002	0.013	0.063

**Table 6. PEI Scores for Process Alternatives<sup>25,49</sup>**

alternative processes ( <i>ij/kj'</i> )	emissions (kg/s) per unit product produced							process PEI per unit product produced
	VOC	CO	NO <sub>x</sub>	PM10	SO <sub>x</sub>	CO <sub>2</sub>	TRS	
TOM (0101)	0.001	0.160	0.158	0.047	0.027	199.600	0.003	0.8971 per klb/s steam
BLGCC (0201)	0.268	4.547	10.320	0.795	0.065	24680.000	0.000	40.33 per MWh/s electricity
DME <sup>a</sup> (0202)	0.015	0.691	0.253	0.062	0.131	305.200	0.000	1.414 per gal/s DME
DME <sup>b</sup> (0203)	0.008	0.117	0.254	0.019	0.203	789.700	0.000	1.271 per gal/s DME
DME <sup>c</sup> (0204)	0.012	0.182	0.421	0.031	0.363	1113.000	0.000	2.083 per gal/s DME
FT <sup>a</sup> (0205)	0.011	0.179	0.464	0.034	0.550	1413.000	0.000	2.511 per gal/s FT
FT <sup>b</sup> (0206)	0.023	0.369	1.002	0.074	1.473	2892.000	0.000	5.698 per gal/s FT
FT <sup>c</sup> (0207)	0.003	0.054	0.146	0.011	0.000	525.000	0.000	0.613 per gal/s FT
mix-alcohol (0208)	0.020	0.316	0.858	0.063	0.136	2861.000	0.000	3.689 per gal/s mix-alcohol

MWh) and sold to the grid,  $C_{\text{elecgrid}}^s$  (\$40/MWh). Note that the latter is lower because of penalties imposed by the electricity supplier.

As the kraft pulp and paper mill requires a huge amount of steam, it is assumed that all steam generated  $T_{\text{steam}}^{\text{Excess}}$  are to be utilized in the pulp and paper mill at price of \$1.534/k lb ( $C_{\text{steam}}^s$ ). To address the energy requirement in this case study, eqs 10 and 11 are revised as follows:

$$T_{\text{elec}}^{\text{Energy}} = \sum_j \sum_i (R_{ij}^I V_{ij\text{elec}}^{\text{EnergyI}}) + \sum_{j'} \sum_k (R_{kj'}^{\text{II}} V_{kj'\text{elec}}^{\text{EnergyII}}) \quad (25)$$

$$T_{\text{elec}}^{\text{Energy}} = T_{\text{elec}}^{\text{Self-consumption}} + T_{\text{elec}}^{\text{Excess}} \quad (26)$$

$$T_{\text{elec}}^{\text{Excess}} = T_{\text{elecmill}}^{\text{Excess}} + T_{\text{elecgrid}}^{\text{Excess}} \quad (27)$$

$$T_{\text{steam}}^{\text{Energy}} = \sum_j \sum_i (R_{ij}^I V_{ij\text{steam}}^{\text{EnergyI}}) + \sum_{j'} \sum_k (R_{kj'}^{\text{II}} V_{kj'\text{steam}}^{\text{EnergyII}}) \quad (28)$$

$$T_{\text{steam}}^{\text{Energy}} = T_{\text{steam}}^{\text{Self-consumption}} + T_{\text{steam}}^{\text{Excess}} \quad (29)$$

As mentioned previously, other than economic performance, environmental performance is also taken into consideration. Tables 5 and 6 show the PEI scores of all the feedstock, products, and the conversion processes that are involved in this case study. Since environmental impact is considered as a conserved quantity,<sup>47</sup> mass balances for the entire process is performed to quantify the flow rates of products and fugitive emissions. The fugitive emissions of the case study are taken from Larson et al.<sup>49</sup> PEI scores for all specified classes of pollutants (i.e., VOC, CO, NO<sub>x</sub>, PM10, SO<sub>x</sub>, CO<sub>2</sub>, and total reduced sulfur), energy (steam and electricity) generated, bioresource (black liquor), intermediate (syngas), and final products (i.e., DME, FT fuel, and mixed-alcohol fuel) are first

quantified using the WAR algorithm as presented previously. For emissions and products that consist of a mixture of chemical components, the PEI score of the mixture is calculated on the basis of its chemical composition and their individual score. For example, the PEI of FT fuel is determined based on the distribution and summation of the individual PEI scores of the hydrocarbon product. The distribution of FT fuel is estimated based on the hydrocarbon product for an Anderson–Schulz–Flory chain-length value of 0.65. As for the environmental impact of each process, the fugitive emissions are given in term of emission factors that are converted into mass flow rates per product basis. Therefore, the PEIs of processes are calculated based on the given emission factor. The categorized emissions from all alternative processes are given in Tables 5 and 6.

In this case study, to accommodate the revenue generated from electricity and steam, eq 12 is revised to eq 30.

$$\begin{aligned} \text{GP} = & \sum_{k'} T_{k'}^{\text{Prod}} C_{k'}^s + T_{\text{elecmill}}^{\text{Excess}} C_{\text{elecmill}}^s + T_{\text{elecgrid}}^{\text{Excess}} C_{\text{elecgrid}}^s + \\ & T_{\text{steam}}^{\text{Excess}} C_{\text{steam}}^s - \left( \sum_i C_i^{\text{Bio}} B_i + \sum_j \sum_i R_{ij}^I V_{ijk}^I C_{ijk}^I + \right. \\ & \left. \sum_k \sum_{j'} R_{kj'}^{\text{II}} V_{kj'k}^{\text{II}} C_{kj'k}^{\text{II}} \right) \quad (30) \end{aligned}$$

It is assumed that the main factor of economic performance is based on GP, thus, eq 13 can be simplified as

$$\text{NPV} = \sum_t^{\text{max}} \frac{(\text{GP} \times A)}{(1 + R)^t} \quad (31)$$

It is further assumed that the annual operating time is given as 8330 h ( $A = 29988000$  s) and the process is designed for an operating life-span of 25 years ( $t^{\text{max}} = 25$ ). However, to limit the complexity of the integrated biorefinery, the maximum number of technologies,  $N_{\text{max}}^{\text{max}}$  is set as two. The expected rate of return,  $R$  is assumed to be 0.15 (15%).

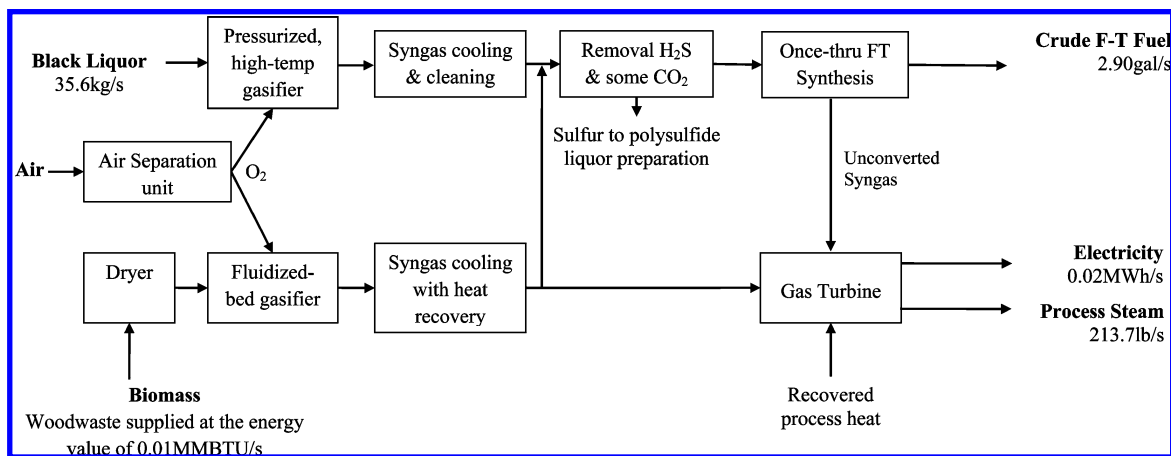


Figure 6. General process flow diagram of the synthesized biorefinery (scenario 1).<sup>25,49</sup>

Meanwhile, environmental performance for the BL biorefinery is measured based on the EPA Waste Reduction Algorithm Graphical User Interface (WAR GUI, build 1.0.17).<sup>25</sup> Each bioresource  $i$  and product  $k'$  are assigned a normalized potential environmental impact (PEI) score, which is obtained from the WAR as  $PEI_i$  and  $PEI_{k'}$ , respectively. These scores represent the relative environmental impact of each species as explained in the previous section. It is noted that a higher negative value of PEI score represent more friendly to the environment and vice versa. In addition, PEI scores for processes  $j$  ( $PEI_{ijk}$ ) and  $j'$  ( $PEI_{k'jk'}$ ) can be determined from the process emissions, utilities consumption and side products based on the detailed data presented in Larson et al.<sup>49</sup> The total potential environmental impact ( $IMP^{Total}$ ) of the synthesized biorefinery can be determined via eq 32 (revised from eq 14) which includes products  $k'$ , process pathways  $j$  and  $j'$ , bioresources  $i$ , and utilities  $e$  (i.e., electricity and steam). Note that the utilities term in eq 14 is replaced by electricity and steam in

$$IMP^{Total} = \sum_{k'} T_{k'}^{Prod} PEI_{k'}^{Prod} + \sum_i \sum_j T_{jk}^{Inter} PEI_{ijk}^I + \sum_k \sum_{j'} T_{k'j'}^{Prod} PEI_{k'j'}^{II} - T_{elec}^{Excess} PEI_{elec}^{Energy} - T_{steam}^{Excess} PEI_{steam}^{Energy} - B_i PEI_{BL}^{Bio} \quad (32)$$

Three different scenarios are considered in this case study, namely, design for maximum economic performance, design for minimum environmental impact, and design considering the conflicting objectives of maximum economic performance and minimum environmental impact via fuzzy optimization.

#### Scenario 1: Design for Maximum Economic Performance.

To synthesize an integrated biorefinery without considering environmental impact, the presented optimization model (eqs 2–9 and 25–32) is solved using the optimization objective in eq 33 and the parameters in Tables 2–5.

$$\text{maximize NPV} \quad (33)$$

The maximum NPV is found as U.S.\$292 million and Fischer–Tropsch synthesis (FT<sup>c</sup>) pathway is selected to produce FT fuel. Besides, the total potential environmental impact,  $IMP^{Total}$  of this process is determined as  $-21.80$ . It is noted that only the single pathway that generates the highest profit is selected. The synthesized configuration is shown in Figure 6. As shown, based on the given feedstock (35.6 kg/s of black liquor), 2.90 gal/s of crude F-T fuel is produced via a high temperature gasifier with oxygen as oxidant and FT synthesis.

Besides, 0.02 MWh/s of electricity and 213.7 lb/s of steam, which supplies the kraft pulp and paper mill, are generated via the gas turbine. Note that the detailed mass and energy balances are not presented in this stage as this optimization model focus on the selection of processes and detailed product allocation.

#### Scenario 2: Design for Minimum Environmental Impact.

In this scenario, the process pathway with minimum environmental impact is determined. To determine the minimum  $IMP^{Total}$ , the objective function given in eq 34 is solved, subjecting to the constraints in eqs 2–9 and 25–32.

$$\text{minimize } IMP^{Total} \quad (34)$$

Based on the optimization result, the minimum  $IMP^{Total}$  is determined as  $-34.06$  and the corresponding NPV is found to be U.S.\$ $-250.24$  million. In this scenario, replacement of the old Tomlinson boiler is recommended to produce electricity and process steam. Based on the conversion table (Table 2) and given feedstock (35.6 kg/s of black liquor), 0.02 MWh/s and 204.7 lb/s of electricity and steam are produced, respectively, to supplement the energy requirement of the kraft pulp and paper mill. Note that in this scenario, the most environmental friendly process generates negative profit. This shows that additional investment is needed to protect the environment.

On the basis of eq 32, a more environmental friendly process can be generated (lower value of  $IMP^{Total}$ ) when black liquor is utilized as feedstock of the black liquor biorefinery or huge amount of energy is exported. This is based on the fact that black liquor is to be discharged to the environment as waste which requires treatment, and all energy requirement of the kraft pulp and paper process is to be sourced externally. Therefore, utilizing black liquor as feedstock of the synthesized biorefinery to generate energy and liquid fuel enables eliminating the discharge of black liquor into the environment and reduce the external energy requirement of the kraft pulp and paper process. Figure 7 shows the synthesized integrated biorefinery that achieves the targeted result.

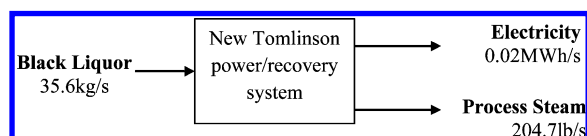


Figure 7. General process flow diagram of the synthesized biorefinery (scenario 2).<sup>25,49</sup>

**Table 7. Fuzzy Goals for Economic and Environmental Performance (Scenario 3)**

fuzzy target	limiting values	
	lower	upper
NPV	$NPV^L = \text{U.S.}\$204 \text{ million}$	$NPV^U = \text{U.S.}\$292 \text{ million}$
$IMP^{\text{Total}}$	$IMP^{\text{Total,L}} = -34.06$	$IMP^{\text{Total,U}} = -21.80$

**Scenario 3: Design Considering the Conflicting Objectives of Maximum Economic Performance and Minimum Environmental Impact via Fuzzy Optimization.** As presented previously, the economic and environmental performances are conflicting with each other, thus, fuzzy optimization is adopted to synthesize the integrated biorefinery. As shown in eqs 22 and 23, upper and lower limits of both objectives are needed. In this case study, the maximum NPV (U.S.\$292 million) generated in scenario 1 is taken as the upper limit of NPV ( $NPV^U$ ). Meanwhile, the minimum environmental impact ( $-34.06$ ), which was obtained in scenario 2, is used as lower limit of  $IMP^{\text{Total,L}}$ . Because the economic analysis metrics remain the predominant tool used in decision making, it has a stricter acceptable fuzzy range with the maximum attainable net present value of U.S.\$292 million as  $NPV^U$  and an acceptable minimum profit as the lower limit,  $NPV^L$ . In this case, it is assumed that the acceptable minimum profit is 30% lower than  $NPV^U$ , which is U.S.\$204 million. It is noted that the acceptable range for the NPV is given by the decision makers and is subject to change on case by case basis. As for the fuzzy range of  $IMP^{\text{Total}}$ , the upper limit ( $IMP^{\text{Total,U}}$ ) is set as the corresponding  $IMP^{\text{Total}}$  when maximum NPV is achieved. Table 7 shows the fuzzy limits for economic and environmental performance targets.

On the basis of the fuzzy goals given in Table 7, eqs 22 and 23 are revised as

$$\frac{NPV - 204}{292 - 204} \geq \lambda \quad (33)$$

$$\frac{-21.8 - IMP^{\text{Total}}}{-21.8 - (-34.06)} \geq \lambda \quad (34)$$

Equation 1 is maximized subject to the constraints in the optimization model (eqs 2–9 and 25–34). The optimization gives an optimum solution with the  $\lambda$  value at 0.1632. The model for this case study has a total of 83 variables and 79 constraints. Figure 8 shows the optimum pathways that satisfied the targeted  $\lambda$ . As shown, BL is first gasified to syngas. Then, the syngas is further processed to DME and FT liquids via pathways DME<sup>b</sup> and FT<sup>c</sup>, respectively. In addition, steam and electricity are being generated and exported to the pulp and paper mill. Table 8

**Table 8. Optimal Results for Black Liquor Biorefinery Case Study (Scenario 3)**

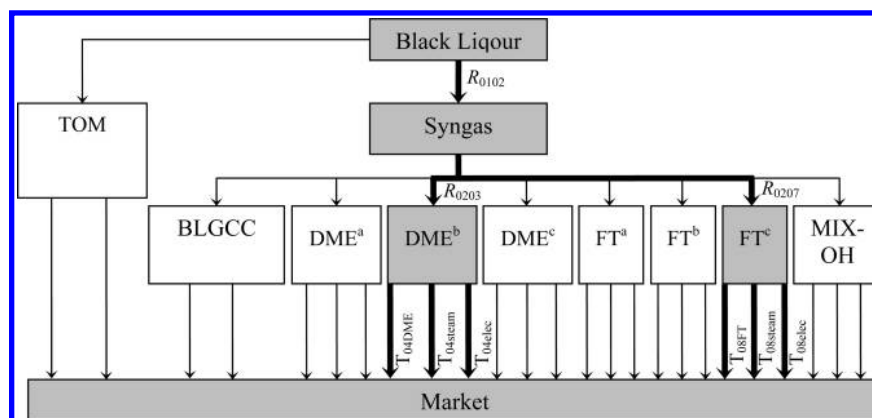
model output	value
NPV	U.S.\$218.42 million
$IMP^{\text{Total}}$	−23.80
DME production rate	0.59 gal/s
FT fuels production rate	2.16 gal/s
total steam production rate	213.7 lb/s
total electricity generation rate	0.02 MWh/s
total electricity sold to the pulp and paper mill	0.02 MWh/s
total electricity sold to the grid	0.00 MWh/s

summarizes the optimum result of this case. It is noted that NPV and  $IMP^{\text{Total}}$  are targeted as U.S.\$218.42 million and −23.80, respectively, with production of 0.59 gal/s DME, 2.16 gal/s FT fuel, 213.7 lb/s steam, and 0.02 MWh/s electricity. Figure 9 shows the final process flow-diagram for the synthesized integrated biorefinery.

### Results Analysis

As shown in literature,<sup>51,52</sup> fuzzy optimization's max–min approach does not guarantee to yield a Pareto optimal solution because of its inability to discriminate between solutions that vary in the attained levels of satisfaction other than the least satisfied goal. Therefore, to ensure the generated result in scenario 3 is located on Pareto optimality, the solution is further analyzed by conducting a Pareto optimality analysis. The fuzzy model is decoupled and solved by setting an incremental value for each of the two objective functions, NPV and  $IMP^{\text{Total}}$ , while maximizing or minimizing the other, to generate the Pareto curve as shown in Figure 10. It is noted that the Pareto solutions are generated on the basis of the constraint that only a combination of two or less technology/technologies is allowed to limit the complexity of the synthesized biorefinery. Note also that the Pareto curve (Figure 10) is generated on the basis of the specific constraints in this case study. Different Pareto-optimal curves can be generated for the model with different constraints (e.g., number of technologies allowed, different fuzzy goals) as specified by decision makers.

As presented previously, a lower  $IMP^{\text{Total}}$  score indicates that a process is more environmentally friendly. As shown in Figure 10, the vertical dotted line at the zero point of NPV represents the edge of the Pareto-optimal curve as processes that generate loss are considered as infeasible options. Note that the individual points in Figure 10 represent the economic and environmental performance of each process available as an option for the integrated biorefinery. In the case where only environmental performance,  $IMP^{\text{Total}}$  is taken into consideration (scenario 2),

**Figure 8.** Optimized pathways that satisfied both economic and environmental performance limits.

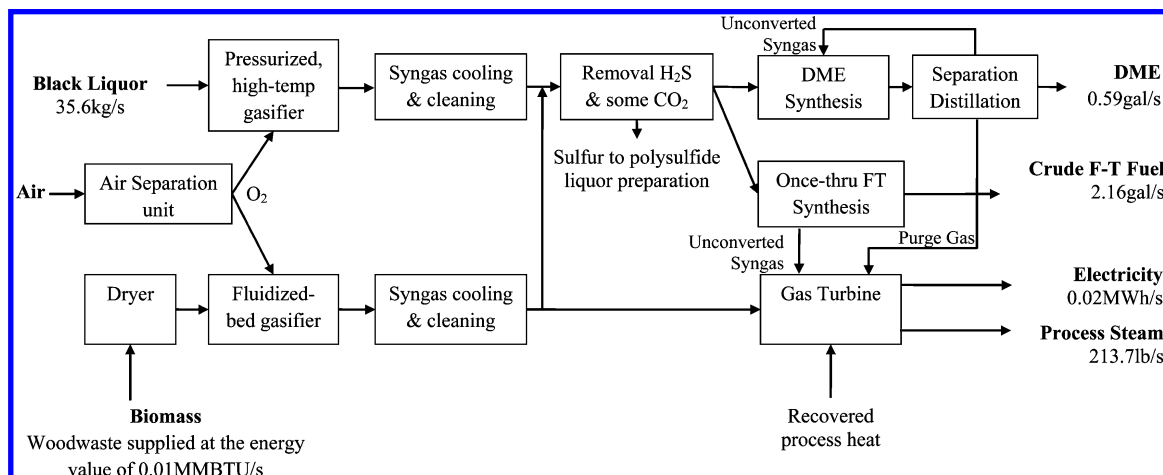


Figure 9. General flow diagram of the synthesized integrated biorefinery with the degree of satisfaction,  $\lambda$  of 0.1632.

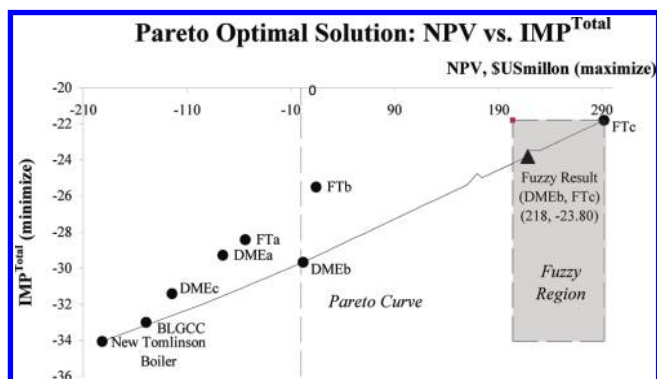


Figure 10. Representation of fuzzy goals and fuzzy optimization results on the Pareto curve.

a new Tomlinson boiler should be installed (Figure 10) to replace the existing Tomlinson boiler. However, this solution will not be accepted by the decision maker because of its poor economic performance.

On the other hand, in case where only NPV is considered, Fischer–Tropsch synthesis with configuration C ( $FT^C$ ) is to be selected. This process yields the highest profit of all the available solutions; however, it has the least desirable environmental impact score. It is worth mentioning that all other available options (i.e., BLGCC,  $DME^c$ ,  $DME^a$ ,  $FT^a$ ,  $DME^b$ , and  $FT^b$ ) are located above the Pareto curve (Figure 10), which are the least preferred domain as they are not the achievable optimal solution available in this system. With the generated Pareto curve in Figure 10, the result from the fuzzy optimization may be visualized. For scenario 3, the fuzzy region is shaded in Figure 10, and the fuzzy optimization result is located within the region. It is interesting to note that a feasible search space (shaded range) is available based on the predefined fuzzy range and the optimized result is located as one of the Pareto optimum solutions.

To demonstrate the feasibility of the optimization model to generate Pareto optimal solutions at other fuzzy goals set by the decision makers, the model is solved with the fuzzy goals as stated and shaded in Table 9 and Figure 11, respectively. In

Table 9. Fuzzy Goals for Analysis of Pareto Optimum Solution

fuzzy target	limiting values	
	lower	upper
NPV	$NPV^L = \text{U.S.}\$0 \text{ million}$	$NPV^U = \text{U.S.}\$292 \text{ million}$
$IMP^{Total}$	$IMP^{Total,L} = -29.50$	$IMP^{Total,U} = -21.80$

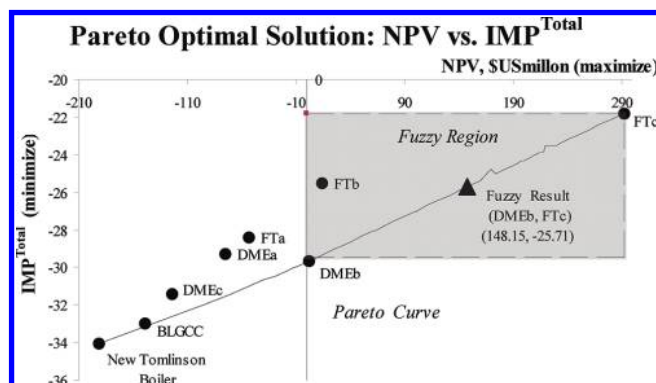


Figure 11. Representation of second fuzzy goals and fuzzy optimization results on the Pareto curve.

Table 10. Optimal Results for Black Liquor Biorefinery Case Study Generated Using Second Set of Fuzzy Goals

model output	value
NPV	U.S.\$148.15 million
$IMP^{Total}$	-25.71
DME production rate	1.15 gal/s
FT fuels production rate	1.46 gal/s
total steam production rate	213.7 lb/s
total electricity generation rate	0.02 MWh/s
total electricity sold to the pulp and paper mill	0.02 MWh/s
total electricity sold to the grid	0.00 MWh/s

this case, the fuzzy goals are set to cover the full spectrum of known feasible Pareto solutions (i.e.,  $NPV > \text{U.S.}\$0 \text{ million}$ ) and its corresponding  $IMP^{Total}$  in the range of  $-21.80$  to  $-29.50$ . The optimization gives a degree of satisfaction,  $\lambda$  at 0.51 which corresponds to NPV of U.S.\$148 million and  $IMP^{Total}$  of  $-25.71$ . The optimized result is summarized in Table 10. As shown, 1.15 gal/s of DME, 1.46 gal/s of FT fuel is produced, while generating 0.02 MWh/s of electricity and 213.7 lb/s of steam. It is assumed that all generated energy is utilized by the kraft pulp and paper mill. As shown in Figure 11, the optimum solution generated by the fuzzy optimization solution is located on the Pareto curve.

Optimization of biorefinery process selection and product allocation using the fuzzy multiobjective approach can generate results more efficiently as compared to a Pareto optimum analysis. This is because an indefinite number of Pareto solution points are required to be generated to sufficiently represent the product allocation of an integrated biorefinery synthesis model. In this case study, a fuzzy multiple-objective optimization



generates a unique optimum solution that matches the result that is generated based on Pareto optimum analysis methodology.

## Conclusion

In this work, fuzzy optimization is extended to products allocation when conflicting objective functions (e.g., economic and environmental performance) are considered. The work is presented as a generic and robust model that allows preliminary synthesis and analysis of integrated biorefineries. An industrial case study was solved to illustrate the proposed approach. These fuzzy extensions are able to account for uncertainties that are often encountered in real-life plant performance analysis and calculation of normalized potential environmental impact score, as well as economic performance. Note that fuzzy optimization is more robust than the crisp optimization with Pareto optimum analysis as no iterative step is required to identify and choose from multiple nondominated solutions. Meanwhile, the case study is used for illustration purpose. The presented generic model can be adapted into different case studies for more detailed analysis.

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## List of Notation

### Sets

- $i$  = index for bioresources
- $j$  = index for technologies/pathways
- $j'$  = index for technologies/pathways
- $k$  = index for intermediates
- $k'$  = index for final products
- $l$  = index for environmental impact categories

### Parameters

- $A$  = annual biorefinery operating time
- $\alpha_l$  = weighting factor of the impact category  $l$
- $C_i^{\text{Bio}}$  = cost of bioresource  $i$
- $C_{ijk}^{\text{I}}$  = processing cost of intermediate  $k$  via pathway  $ij$
- $C_{kj'k'}^{\text{II}}$  = processing cost of intermediate  $k'$  via pathway  $kj'$
- $C_k^{\text{Prod}}$  = revenue from product  $k'$
- $C_e^{\text{Energy}}$  = revenue from exported energy streams (e.g., steams, electricity, etc.)
- $C_{\text{elec}^{\text{mill}}}^{\text{s}}$  = revenue from electricity exported to the kraft pulp and paper mill
- $C_{\text{elec}^{\text{grid}}}^{\text{s}}$  = revenue from electricity exported to the grid
- $C_{\text{steam}}^{\text{s}}$  = revenue from steam exported to the pulp and paper mill
- DEP = depreciation
- GOV = government incentives or penalties
- HEDGE = expenses associated with hedging against catastrophic market actions
- $\text{IMP}^{\text{Total,L}}$  = lower limit of total potential environmental impact score
- $\text{IMP}^{\text{Total,U}}$  = upper limit of total potential environmental impact score
- $N_j^{\text{I max}}$  = maximum number of potential pathway/technology  $j$
- $N_{j'}^{\text{II max}}$  = maximum number of potential pathway/technology  $j'$
- $\text{EP}^{\text{L}}$  = lower limit of economic performance
- $\text{EP}^{\text{U}}$  = upper limit of economic performance
- $\text{NPV}^{\text{L}}$  = lower limit of net present value
- $\text{NPV}^{\text{U}}$  = upper limit of net present value
- $R$  = expected rate of return or cost of capital
- $t^{\text{max}}$  = designed lifespan of the biorefinery

TAX = marginal tax rate

$V_{ijk}^{\text{I}}$  = conversion of bioresource  $i$  to intermediate  $k$

$V_{ije}^{\text{Energy I}}$  = conversion of utilities per unit of bioresource  $i$  via technology/pathway  $j$

$V_{kje}^{\text{Energy II}}$  = conversion of utilities per unit of intermediate  $k$  via technology/pathway  $j'$

$V_{j\text{steam}}^{\text{Energy I}}$  = conversion of steam per unit of bioresource  $i$  via technology/pathway  $j$

$V_{kj\text{steam}}^{\text{Energy II}}$  = conversion of steam per unit of intermediate  $k$  via technology/pathway  $j'$

$V_{jelec}^{\text{Energy I}}$  = conversion of electricity per unit of bioresource  $i$  via technology/pathway  $j$

$V_{kjelec}^{\text{Energy II}}$  = conversion of electricity per unit of intermediate  $k$  via technology/pathway  $j'$

$V_{kj'k'}^{\text{I}}$  = conversion of intermediate  $k$  to product  $k'$

PEI = potential environmental impact score

$\text{PEI}_b$  = potential environmental impact score of chemical  $b$

$\text{PEI}_{b-l}$  = weighted average potential environmental impact score of chemical  $b$  in category  $l$

$\text{PEI}_{\text{Bio}}^{\text{Bio}}$  = potential environmental impact of black liquor

$\text{PEI}_e^{\text{Energy}}$  = potential environmental impact of utilities  $e$

$\text{PEI}_{\text{elec}}^{\text{Energy}}$  = potential environmental impact of electricity

$\text{PEI}_i$  = potential environmental impact score of bioresource  $i$

$\text{PEI}_{ijk}^{\text{I}}$  = potential environmental impact score of technology/pathway  $j$

$\text{PEI}_k^{\text{Prod}}$  = potential environmental impact score of product  $k'$

$\text{PEI}_{kj'k'}^{\text{II}}$  = potential environmental impact score of technology/pathway  $j'$

$\text{PEI}_i^{\text{Bio}}$  = potential environmental impact of bioresource  $i$

$\text{PEI}_{\text{steam}}^{\text{Energy}}$  = potential environmental impact of steam

### Variables

NPV = net present value

$B_i^{\text{Bio}}$  = flow rate of bioresource  $i$

GP = gross profit per unit time

$dI_{\text{system}}/dt$  = change in system environmental impact over time

$I_j^{\text{I}}$  = binary integer for technology/pathway  $j$

$I_{j'}^{\text{II}}$  = binary integer for technology/pathway  $j'$

$i_{\text{in}}$  = input rates of impact entering the process

$i_{\text{out}}$  = output rates of impact leaving the process

$i_{\text{gen}}$  = environmental impact generated within the system

$dI/dt$  = accumulation (or depletion) of environmental impact in the given system over time

$i_{\text{in}}^{(\text{cp})}$  = input rates of impact in the chemical process

$i_{\text{out}}^{(\text{cp})}$  = output rates of impact in the chemical process

$i_{\text{in}}^{(\text{ep})}$  = input rates of impact in the energy generation process

$i_{\text{out}}^{(\text{ep})}$  = output rates of impact in the energy generation process

$i_{\text{we}}^{(\text{cp})}$  = impact generated from the release of waste energy to the environment from chemical processes

$i_{\text{we}}^{(\text{ep})}$  = impact generated from the release of waste energy to the environment from energy generation process

$i_{\text{gen}}^{(\text{I})}$  = impact generated by chemical reactions within the system

$M_a^{\text{out}}$  = mass flow rate of stream  $a$  leaving the process

$M_a^{\text{in}}$  = mass flow rate of stream  $a$  entering the process

$x_{b-a}$  = mass fraction of a given chemical  $b$  in stream  $a$

$\text{IMP}^{\text{Total}}$  = total potential environmental impact score

$R_i^{\text{I}}$  = flow rate of bioresource  $i$  to technology/pathway  $j$

$R_{kj'}^{\text{II}}$  = flow rate of intermediate  $k$  to technology/pathway  $j'$

$T_k^{\text{inter}}$  = total production rate of intermediate  $k$

$T_k^{\text{Prod}}$  = total production of product  $k'$

$T_e^{\text{Energy}}$  = total production of utilities

$T_e^{\text{self-consumption}}$  = total utilities requirement of the synthesized integrated biorefinery  
 $T_e^{\text{excess}}$  = excess energy that are sold to the grid or any third party plants  
 $T_{\text{elec}}^{\text{Energy}}$  = total production of electricity  
 $T_{\text{elec}}^{\text{self-consumption}}$  = total electricity requirement of the synthesized integrated biorefinery  
 $T_{\text{elec}}^{\text{excess}}$  = excess electricity that are sold to the grid or any third party plants  
 $T_{\text{elec}}^{\text{excessmill}}$  = excess electricity that are exported to the kraft pulp and paper mill  
 $T_{\text{elec}}^{\text{excessgrid}}$  = excess electricity that are exported to the grid  
 $T_{\text{steam}}^{\text{Energy}}$  = total production of steam  
 $T_{\text{steam}}^{\text{self-consumption}}$  = total steam requirement of the synthesized integrated biorefinery  
 $T_{\text{steam}}^{\text{excess}}$  = excess steam that are sold to any third party plants  
 $\lambda$  = degree of satisfaction of fuzzy goals

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