Multi-objective optimal synthesis of algal biorefineries toward a sustainable circular bioeconomy

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Abstract. Production of biodiesel from renewable resources like microalgae biomass presents a potential for reduction of greenhouse gas emissions and fossil fuel energy consumption. The integration of processes from other industries has been implemented in microalgal biorefineries to increase economic sustainability by co-producing several high-value algal-based products. Agro-industrial processes have the potential to be incorporated into the biorefinery because it requires input material flows from other biorefinery process units to cultivate and sell crops for an additional source of revenue and increased carbon sequestration, while generating wastewater that may be used as a cultivation medium for algae or as a resource for other biorefinery processes. Circular bioeconomy, an extension of the circular economy ideology, has the goal of achieving economic and environmental sustainability through maximizing the dedicated recirculation of resource flows, and minimizing waste generation and end-of-life disposal. However, existing modelling studies have not explored this opportunity; previous studies have not considered that resource functionality runs out with repeated recirculation and reuse as it reaches its end of life. In this work, a novel multi-objective optimization model is developed to design and manage closed-loop algal biorefineries integrating agro-industrial processes that captures the effect of recirculation on resource material viability and end-of-life environmental impact. A case study is solved as proof of concept and to illustrate the design methodology, optimal solutions based on economic and environmental performance are analyzed. The results of the case study validate the initial hypothesis that there is a conflict between the economic and environmental objectives since the decision for biofuel production varied for each single objective. With the multi objective model, a balance between the two objectives was found. The results of the optimization model can be applied in the design of an algal biorefinery along with the decisions relating to production quantities incorporating a zero waste outlook.

1. Background

Environmental concerns have been arising with the diminishing supply of fossil fuels coupled with the rise of greenhouse gas emissions heavily influenced by its production and energy consumption. With that, it is essential to look into the utilization of renewable energy sources as sustainable alternatives. Microalgae, due to its higher photosynthetic efficiency [1, 2], higher growth productivity [3, 4], and high lipid content [5, 6], is considered as one of the most valuable feedstock for the production of biofuel. Microalgae can seize carbon dioxide from the atmosphere which then allows the production process of
biodiesel to be carbon neutral [7, 8]. However, the viability of microalgal biofuels as an alternative energy source faces economic challenges as it competes with the relatively inexpensive production costs of fossil fuels.

Integrated approaches are necessary to be able to maximize biomass utilization for the entire value chain [9, 10]. Algal biorefinery facilities are constructed to produce bioenergies in conjunction with various bioproducts from algal biomass. Bioenergies are low-value, but high-volume biofuels and include biodiesel, bioethanol and biogas, to name a few. Bioproducts generally have a high value, although usually recovered in low volumes, which can include biopharmaceuticals, biochemicals, and biofertilizers. These high-value products provide higher profitability and biomass efficiency for the biorefinery. Total chain integration of biorefineries have the potential to minimise costs, maximise quality and quantity of biorefinery end products as well as lessen environmental impacts and enhance societal benefits [11]. With that, numerous studies have looked into the possible integration for biorefineries aiming to establish a zero waste process flow for biofuel production. However, these studies that have tackled the optimization of processes in an integrated algal biorefinery have certain limitations in terms of environmental considerations with the aim of a circular bioeconomy. On the other hand, these limitations have been addressed in several conceptual model proposals for integrated algal biorefineries. Galanopoulos et.al and García Prieto et.al formulated optimization models with a single objective of cost minimization and profit maximization respectively. However, it is apparent that environmental impact must be considered when looking into the optimization of an algal biorefinery to yield the most sustainable results. This has been addressed by Sy et.al who included various environmental footprints into the optimization model such as carbon, water, land, nitrogen and phosphorus when assessing the integrated algal biorefinery. Despite this, the previously mentioned studies failed to look into the integrated algal biorefineries at a closed loop approach. Wu & Chang proposed a methodology making use of life cycle assessment (LCA) and techno-economic assessment (TEA) methods aimed as input for a multi-objective linear programming model to optimize processes in a closed loop algal biorefinery. However, this study simply reviewed an integrated algal biorefinery with a zero waste concept and provided a methodology for multi-objective optimization.

Therefore, a mathematical optimization model must be developed centered on an algal biorefinery that simultaneously optimizes cost and environmental impact, integrates agro-industrial inputs and processes aimed toward a closed loop process flow, and incorporates the life cycle assessment methodology to properly consider the environmental footprints of the integrated algal biorefinery.

2. System Definition

The integrated algal biorefinery is composed of \( i \) process units and makes use of \( j \) number of raw material and energy streams. These streams then serve as the values for process matrix \( A_{ij} \) wherein columns represent the \( i \) process units and rows represent the \( j \) material and energy streams. Negative values in the \( A_{ij} \) matrix states that the stream serves as an input to the process unit while positive values indicate that the stream is an output of the process. Demand for each product output \( j \) is represented by \( D_j \). Variable costs \( (VC_j) \) are associated with each raw material and energy stream as well as selling prices \( P \) for each product stream \( y_{ij} \). Moreover, fixed costs are also assigned to each process unit \( i \), defined by the variable \( FC_i \).

The environmental impact values used for the minimization objective are retrieved through the life cycle assessment methodology. The goal of the study is to evaluate the overall environment impacts of the integration of various process units yielding multiple co-products for a microalgal biorefinery. The system boundary of the study is shown in Figure 2. The upstream and downstream processes are segregated to represent the different parts of the microalgae life cycle which are the cultivation & extraction phases and the preparation & production phases. Aside from that, this study will also look into the use & disposal scenarios of each biorefinery product. The functional unit for LCA normalization to be used in this model would be 1 kg of biodiesel of the microalgae biorefinery, the selection of which will be obtained from the results of the linear programming model. In retrieving the environmental impact assessment for the algal biorefinery, \( k \) impact categories are looked into to evaluate the process.

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systems. These environmental impacts from each category associated to each algal biorefinery process unit are then represented by the parameter $E_k$. To develop a single score evaluation for the entire process system as defined by the variable $S_n$, weights ($W_k$) are assigned for each environmental impact category.

### 3. Model Formulation

The overall objectives of the mathematical optimization model are profit maximization and environmental impact minimization represented by Equations (1) and (2). The profit is the difference between the sales from all products and the total costs generated by the biorefinery which are the purchase costs of raw material and energy streams and the fixed costs of each process unit utilized. The environmental objective is simply the overall single score impact for the entire process system which is computed by multiplying the single score for each unit output of the processes by the total output of each process unit.

$$\text{Profit} = \sum_i P_i y_{ij} - \sum_i V_i C_i x_{ij} - FC_i b_i$$ (1)

$$\text{Impact} = \sum_j S_j y_{ij}$$ (2)

Given that the model has two objectives, a balance must be realized between the two to obtain the optimal solution. With that, the objective function is then set to the maximization of the least desirability value to strike a balance between the two objectives as seen in Equation (5) [12]. The efficiency values are calculated by ratio of the obtained improvement, which is actual value subtracted from the worst, and the potential improvement, which is the potential value subtracted from the worst possible as shown in Equation (3) & (4). The potential values for the profit and impact objectives are attained by the optimization of each corresponding objective applied into a single objective mathematical model. It is assumed that the worst possible result that the environmental impact may yield is the corresponding value when the optimization for the profit is executed, and vice versa.

$$\text{Eff}_\text{Profit} = \frac{\text{Profit}_{\text{worst}} - \text{Profit}}{\text{Profit}_{\text{best}} - \text{Profit}_{\text{worst}}}$$ (3)

$$\text{Eff}_\text{Impact} = \frac{\text{Impact}_{\text{worst}} - \text{Impact}}{\text{Impact}_{\text{best}} - \text{Impact}_{\text{worst}}}$$ (4)

$$\text{Maximize } Z = \min [\text{Eff}_\text{Profit}, \text{Eff}_\text{Impact}]$$ (5)

Given that the objective function presented above is nonlinear, linearizing constraints are necessary to ensure that the optimization solver can obtain the solution to the model. The constraints are presented in Equations (7) & (8) below which indicate that the overall efficiency, $Eff$, obtains a value equal to the minimum of the two efficiencies, $Eff_{\text{Profit}}$ and $Eff_{\text{Impact}}$.

$$\text{Maximize } Z = Eff$$ (6)

$$Eff \leq Eff_{\text{Profit}}$$ (7)

$$Eff \leq Eff_{\text{Impact}}$$ (8)

The constraints of the mathematical model involve the input and output material balancing for each process unit, incorporating a circular bioeconomy outlook.

$$\gamma_j = \sum_i A_{ij} x_{ij} \quad \forall j$$ (9)

$$\gamma_j - \sum_i x_{ij} \geq D_j \quad \forall j$$ (10)

Equation (9) represents the relationship between the process outputs $y_j$ for each material $j$ which is calculated by multiplying the process matrix $A_{ij}$ with the material stream vector $x_{ij}$. The total material
process inputs \( x_{ij} \) for each material \( j \) is subtracted from the total process outputs of material \( j \) represented by \( y_j \), which is then set to be greater than or equal to the product demand vector \( D_j \) as presented in Equation (10). This is done to indicate that the model will only generate process outputs that will either be used to satisfy a given demand or used in a different process unit for a zero-waste process system.

\[
\begin{align*}
\sum_j x_{ij} & \leq Mb_i \quad \forall i \\
S_i & = E_{ik}W_k \quad \forall i
\end{align*}
\]

Equation (11) represents the constraint involving the relationship between the binary variable for the process units \( b_i \) and its corresponding material stream inputs \( x_{ij} \) where \( M \) corresponds to an arbitrary large number. The last two constraints involve the boundaries of the decision variables. The calculation formula for the single score vector \( S_i \), which is the product of the environmental impact vectors for each process unit \( i \) output and impact category \( k \) with their corresponding weights as represented in Equation (12).

\[
\begin{align*}
x_{ij}, y_j & \geq 0 \quad \forall i \forall j \\
b_i & \in \{1,0\} \quad \forall i
\end{align*}
\]

The process input vector \( x_{ij} \) as well the output vector \( y_j \) should be nonnegative to represent the chosen capacity of each process unit as shown in Equation (13). Equation (14) presents the nature of a binary variable which can obtain a value of either one or zero.

4. Model Validation
The mathematical model optimization procedure is implemented using the MATLAB software using the Cplex optimization solver. A base scenario is initially considered as a foundation for comparison of the following problem scenarios. The base scenario assigns equal weights for all environmental impact categories in vector \( W_k \). To generate the worst and best possible results regarding the two objectives to be used in the computation for efficiency, single objective optimization is done for profit and environmental impact. A case study involving a microalgal bio refinery with biochar production, anaerobic digestion, combined heat and power, and transesterification as its downstream processes is developed to validate the linear programming model.

| Table 1. Summary of mathematical model results for each objective |
|---------------------------------------------------------------|
| **Profit (in USD)** | 2605864.39 | 1890757.13 | 1892628.00 | 99.7% |
| **Impact (kg CO2)** | 1.08895E-08 | 1.59397E-05 | 4.78519E-08 | 99.7% |

Considering the economic profit objective only, the biochar production process unit as well as the anaerobic digestion and combined heat and power units were maximized to produce the most output catering to the demand. With a zero-waste objective, all wastes were utilized in consequent processes such as algal residue being converted to liquid and solid residue which is then converted to methane gas turning into power and heat, and biochar which can be used as fertilizer.

Looking into the use of the environmental impact objective, process units were not used up as much and were only utilized to meet the set demand. This is because the environmental impacts retrieved from the life cycle assessment study had high consideration of the impact per unit output of each process unit. With that, the combined heat and power unit was not completely utilized at all since the power and heat it produces will yield a significantly high amount of environmental impact.
Utilizing the economic and environmental objectives in the mathematical model simultaneously, the resulting value for the profit was not far from the worst case scenario for the profit. However, for the environmental impact objective, it is very much near the best case. This indicates that in satisfying the multi-objective optimization model objectives and constraints, the model leaned towards the environmental aspect more than the economic considerations.

5. Conclusions and Recommendation
A mathematical optimization model centered on an algal biorefinery that simultaneously optimizes cost and environmental impact, integrates agro-industrial inputs and processes aimed toward a closed loop process flow, and incorporates the life cycle assessment methodology to properly consider the environmental footprints of the integrated algal biorefinery is developed in this study. The maximization of efficiencies based on the best and worst possible results regarding the profit and environmental impact objective is made to determine the optimal solution. The optimization model is validated using a case study involving an algal biorefinery with biochar production, anaerobic digestion, combined heat and power, and transesterification as its downstream processes. Having optimized the two objectives separately, displayed the tradeoffs that occur between the environmental and economic objectives. When profit is maximized, conflict is evident as the environmental impact increases. With the implementation of impact minimization, yields a net loss for the algal biorefinery given that less revenue is generated due to lowered biofuel production. The consideration of both objectives in a multi-objective optimization model strikes a balance between the two objectives.

The results of the optimization model can then be applied by project managers in the design of an algal biorefinery along with the decisions relating to production quantities. Future work may look into the incorporation of different methodologies to determine the most appropriate weights to be given to the various environmental impacts. Moreover, the integration of uncertainty regarding process outputs and demand quantities is a possible extension of this research given that variations in demand and process outputs directly relate to the optimal results generated from the model. Lastly, the use of real-life data for the estimation of parameters in the model would likely yield more appropriate results to be applied in real-world industry applications.

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