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A Mixed-Integer Dynamic and Stochastic Algae Process Optimization

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Abstract: With increased energy demand as it gets scarcer, a great deal of research is being carried out into alternatives to non - renewable energy resources. One of the promising studies is the biofuel production from micro algae. Microalgae are photosynthetic organisms and capture carbon dioxide, reducing emissions and providing valuable products (fuel, fertilizer, etc.). Thus, efficiency in the design and optimization of process related units are important. In this study, the optimal experimental conditions for *Nannochloropsis Oculata* were calculated under the constraints of the model equations and other process related constraints through simultaneous optimization approach. The economic evaluation of the process is also handled by introducing the uncertainty in the economic measures sampled from normal distribution to maximize the average profit. Unlike traditional approaches, the MINLP formulation, which is solved stochastically, dynamically, and simultaneously, provides more robust and reliable results, flexibility, improved decision making, reduced risks to be taken and a better understanding of risk factors.

Keywords: Stochastic Optimization; MINLP; Dynamic Optimization

1. INTRODUCTION

Today, we are questioning our dependence on traditional fossil fuels and turning to alternative energy sources as the world's energy needs continue to grow. In this regard, environmental sustainability and clean energy production are becoming increasingly important. Renewable sources of energy are one of the solutions to these challenges. Biomass is a group of sources that stands out among these renewable energy sources and offers several advantages. It interferes less with natural cycles and reduces the amount of greenhouse gases released into the atmosphere.

The energy obtained from biomass is considered to be an effective strategy in the fight against climate change. Additionally, biomass resources contribute not only to energy production but also to waste management, providing both environmental and economic benefits through the conversion of organic waste into energy. Third generation biomass resources are obtained using advanced technologies such as genetic engineering and biotechnology to increase biomass production. They are highly efficient and have a significant carbon dioxide absorption ability, making them a reliable and sustainable source of energy production while minimizing environmental impacts (Behera et al., 2015).

Microalgae can be used to produce valuable biochemicals, including biodiesel, bioethanol, and biogas, with high efficiency using solar energy. In addition to their unique properties, microalgae offer several benefits, such as efficient wastewater management and carbon capture and storage. These advantages make microalgae a sustainable bioenergy source that can play an important role in both energy production and the production of valuable biochemicals.

In order to fully evaluate the potential of microalgae for bioenergy production, it is important to conduct optimization studies that focus on the solution of existing problems. Specifically, the reduction of energy consumption and cultivation costs will make microalgae bioenergy production more competitive. Through these studies, microalgae can become a more widely used and sustainable energy source. Therefore, it is crucial to support the ongoing research and development efforts for the more widespread use of microalgae in the bioenergy sector. This will help us to take important steps towards a clean and sustainable energy future.

Mixed Integer Nonlinear Programming (MINLP) has a wide range of potential applications in engineering, mathematics, and operations research. This method works with complex mathematical expressions that include both continuous and discrete variables. It often includes nonlinear objective functions and/or constraints. Continuous variables are

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commonly used to represent continuous conditions such as temperature, pressure, concentration, or flow. Discrete variables are often defined as binary variables to represent presence or absence. MINLP is a powerful tool that has been effectively used in engineering and planning areas such as process synthesis, process control, process design selection, process scheduling, and site selection. For solving complex engineering problems, it is considered to be particularly useful. Thus, MINLP has become a popular choice for finding optimized solutions in engineering and planning disciplines (Biegler, 2010; Floudas, 2000). Even apparently simple systems can display intricate interactions in models with various constraints and objective functions. This implies that conventional methods may not suffice for analyzing and optimizing systems. Therefore, utilizing the MINLP (Mixed Integer Nonlinear Programming) formulation allows for a simultaneous optimization study by considering different types of constraints and objectives together. This approach enables a more comprehensive understanding of the system's holistic structure and facilitates the attainment of a global solution. Therefore, utilizing the MINLP formulation for such analyses can assist in achieving more robust and comprehensive results.

Dynamic optimization problems are a broad class of problems that frequently involve extensive sets of differential algebraic equations, complex control, and constraints on state variables. They provide a mathematical framework for understanding and optimizing how the system will behave over time. Advances in technology and mathematics, along with increased computational capabilities, have enabled the use of powerful and modern tools for formulating and solving dynamic optimization problems (Laiglecia et al., 2013).

Dynamic optimization plays a critical role in many fields, including chemical engineering, pharmaceuticals, value-added synthesis, and specialty chemicals. In this context, optimizing process parameters using this frequently preferred approach is common in modeling batch and semi-batch reactors. This method has the capacity to increase process efficiency, reduce costs, and maximize the desired product quantity.
Many processes, including bioprocesses, exhibit nonlinear dynamics and require dynamic optimization methods to determine optimal process conditions. This is particularly important in fields such as biotechnology, the food industry, and biofuel production. Dynamic optimization is considered a crucial tool for managing and optimizing complex systems. Its effectiveness and usage are increasing due to advancements in technology and mathematics. (Banga et al., 2005; Laiglecia et al.,2013).

In contrast to deterministic approach, models that deal with uncertainty are crucial in performing optimization under uncertain conditions (Henrion et al., 2001). While deterministic optimization operates with certain values, stochastic optimization considers uncertainties and accounts for the discrepancies in actual values. There are various sources of uncertainty in chemical and bioprocesses, including raw material costs, product purity, demand from consumers, reactor and catalyst efficacy. Thus, it is crucial to employ stochastic modelling in the analysis of process systems (Sharifian et al., 2021).
In this study, the dynamic optimisation of *Nannochloropsis Oculata* algae growth, calculating optimal process conditions and maximising biomass profit under economic uncertainty was analysed, and the effect of dynamic and non-linear constraints on the process were also investigated. For realistic modelling and optimisation of complex systems and processes, the addition of a stochastic model to mixed integer nonlinear dynamic models offers significant advantages.

This approach provides a means of understanding process dynamics and variability in detail through dynamic models. Furthermore, this combination can respond more effectively to uncertainties, dynamic changes, and complex integer constraints in business processes. At the same time, this approach promotes continuous improvement by providing a more robust framework for system optimisation, risk analysis and decision-making strategies.

2. METHODOLOGY

This study aims to develop a stochastic MINLP model for *Nannochloropsis Oculata* algae by updating Tijani et al.'s previous model (Tijani et al., 2018). The mathematical model which aims to maximize the avarage profit of all scenarios is given by:

$$\max_{X,P,N,CO_2,C_x,\mu_x,b_i,r_i,h_i,F_i} \frac{\sum_{s=1}^{s_T}(R[s]-E[s])}{s_T}$$

$$\begin{aligned} R[s] &= X(t_f)\cdot\left(\sum_{i=1}^{5} b_i V_{r,i}\right)\cdot\left(p_f[s]\cdot f_f[s]+p_{fr}[s]\cdot f_{fr}[s]\right) \\ E[s] &= X(t_f)\cdot\left(\left(\sum_{i=1}^{5} b_i V_{r,i}\right)\cdot\left(\sum p_{oc}[s]\right) + \left(p_w[s]\cdot\sum_{i=1}^{5} b_i V_{r,i}\right)\right) \end{aligned} \tag{1}$$

$$subject\ to:$$

$$\mu_x(t) = \mu^{max}\cdot\phi\cdot(\alpha\cdot\mu_N(t)+\beta\cdot\mu_P(t)+\delta\cdot\mu_C(t))$$

$$\mu_N(t) = \left(\left[1-\frac{k_N}{[N(t)]}\right]\cdot\frac{[X(t)]}{\varphi_N} - \frac{\sum_{i=1}^{5}(b_i D_i)}{\mu^{max}}[N(t)]\right) \tag{2}$$

$$\mu_P(t) = \left(\left[1 - \frac{k_P}{[P(t)]}\right] \cdot \frac{[X(t)]}{\varphi_P} - \frac{\sum_{i=1}^{5}(b_i D_i)}{\mu^{max}} [P(t)]\right)$$

$$\mu_C(t) = k_l \cdot a \cdot \frac{[CO_2(t)]\left(1 - \sum_{i=1}^{5}(b_i D_i)\right) - [C_x(t)]}{\mu^{max}} - \left[1 - \frac{k_C}{[CO_2(t)]}\right] \cdot \frac{[X(t)]}{\varphi_{co2}}$$

$$\frac{dX}{dt} = \mu_X(t) \cdot [X(t)] - \sum_{i=1}^{5}(b_i D_i) \cdot [X(t)]$$

$$\frac{dC_x}{dt} = 0$$

$$\frac{dP}{dt} = -\mu_X(t) \cdot \frac{[X(t)]}{\varphi_p} - \sum_{i=1}^{5}(b_i D_i) \cdot [P(t)]$$

$$\frac{dCO_2}{dt} = \gamma \frac{dX}{dt}$$

$$\frac{dN}{dt} = -\mu_X(t) \cdot \frac{[X(t)]}{\varphi_N} - \sum_{i=1}^{5}(b_i D_i) \cdot [N(t)]$$

$$\sum_{i=1}^{5} b_i = 1$$

$$V_i = \pi r_i^2 h_i$$

$$D_i = F_i / V_i$$

$$\mu^{max} \geq \mu_x(t)$$

$$r_{i,min} \leq r_i \leq r_{i,max}$$

$$h_{i,min} \leq h_i \leq h_{i,max}$$

$$\frac{r_i}{h_i} \geq 0.25$$

$$\frac{r_i}{h_i} \leq 0.9$$

Additional constraints are given by:

$$X(0) = 0.100$$

$$N(0) = 0.290$$

$$0.2 \leq CO_2(t)$$

$$0.25 \leq C_x(t)$$

$$P(0) = 0.049$$

$$CO_2(0) = 0.317$$

where s and s_T are the number of the scenario and total number of scenarios respectively; $R[s]$ is the revenue and calculated using fuel sales price, $p_f[s]$, fuel sales factor, $f_f[s]$, fertilizer sales price, $p_{fr}[s]$, and fertilizer sales factor $f_{fr}[s]$; $E[s]$ is expense; $p_{oc}[s]$ represent operating costs; $p_w[s]$ is water price; μ^{max} represents the maximum biomass specific growth rate under specified conditions; the specific rates of growth μ_N, μ_P and μ_C denote nitrogen-limited, phosphorus-limited, and carbon-limited conditions; k_i is limiting cell quota for each component (nitrogen, carbon dioxide, phosphorus); X, N, P are concentrations of biomass, nitrogen, and phosphorus, respectively; CO_2 and C_x represent the liquid phase carbon dioxide concentration in culture medium and the free carbon dioxide in the medium which is not use in cultivation ; γ_i is yield coefficient of components; k_l is the overall mass transfer coefficient for CO_2 injection to liquid medium and a is cell surface area per volume (m^{-1}); $k_l.a$ the coefficient a was limited to the range of (107-156) d^{-1} based on the experimental data by Tijani et al., (2018); α, β and δ are weighting factors and determine as 0.197 0.079 and 0.441 respectively by (Tijani et al., 2018); ϕ is a tuning parameter to account for the impact of light and depends on numerous factors such as the length of the light path coming from the surface, the average absorption coefficient, the biomass concentration, the intensity of the incident light and the instantaneous light intensity in the range of 0.58-0.91 and should be obtained from experimental data; b_i are the binary variables for the selection of one of five available reactor sizes; $X(0), N(0), P(0)$, and $CO_2(0)$ are initial concentrations of biomass, nitrogen, phosphorus and carbon dioxide, respectively. $fuel_f[s]$ and $fert_f[s]$ account for losses due to separation process after the reaction and assumes only 30% of the biomass is converted into fuel and fertilizer, respectively. $r_{i,min}$, $h_{i,min}$ and $r_{i,max}$, $h_{i,max}$ represent upper and lower limits reactor radius and height for each reactor *"i."*

In this study, it was assumed that the amount of carbon dioxide in the cultivation medium would remain constant. The main reason for this assumption is the presence of a fixed and continuous carbon source in the cultivation medium, so it is predicted that the carbon dioxide concentration will also remain constant. In calculating the initial values of the differential equations expressing nutrient and carbon concentrations, the optimum values were calculated by determining the lower and upper limit constraints and these values were then fixed. Experimental parameter values were calculated using theoretical data from Tijani et al. The calculations were based on minimizing the square of the difference between experimental and theoretical data through regression analysis (see Appendix A). The parameter values were subject to certain constraints to ensure model accuracy and consistency. Thus, the calculated parameter values are defined as model parameters determined through regression analysis.

The optimization problem is solved by using Basic Open-source Nonlinear Mixed-Integer programming (BONMIN) solver which is capable for Mixed Integer Quadratically Constrained Programs (MIQCPs) and MINLPs. Parameter values which are used in mathematical model are given in Table 1:

Table 1. Growth Parameter Values

Parameter	Value	Unit
μ^{max}	0.3110	d^{-1}
k_N	0.0417	kgN/m^3
φ_N	851.81	kgX/kgN
k_P	0.0006	kgP/m^3
φ_P	192.92	kgX/kgP
k_C	0.2862	$kgCO_2/m^3$
φ_{co2}	0.0082	$kgX/kgCO_2$
$k_l \cdot a$	127.64	d^{-1}
D_1	0.1000	d^{-1}
D_2	0.0800	d^{-1}
D_3	0.0900	d^{-1}
D_4	0.1100	d^{-1}
D_5	0.1200	d^{-1}
α	0.1970	--
β	0.0790	--
δ	0.4410	--
ϕ	0.8570	--
γ	0.0890	--

3. RESULTS

Algae growth profile under consideration includes a 12-day exponential growth period ended due to extinction of substrate. Fig. 1 is obtained through a deterministic approach where the economic considerations are fixed (Kivanc et al.,2023).

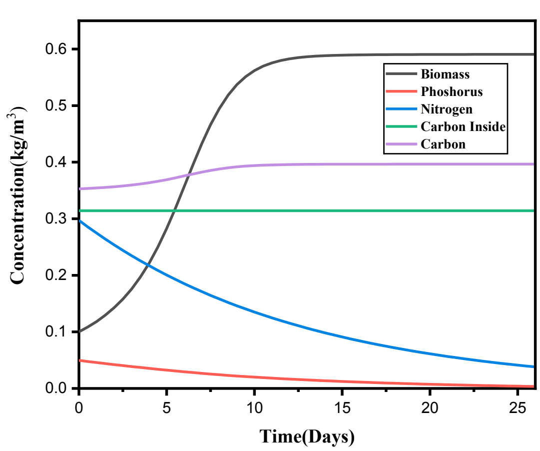

Figure 1. Concentration Profiles of Nutrients and Biomass.

Table 2 and 3 display the computed results for each case of the simulation study based on the reactor dilution coefficient. The analysis indicates that low dilution coefficients and high reactor volumes are the optimum reactor operation parameters. Moreover, the low dilution coefficient operations accomplished maximum biomass concentration. Upon examination of the gathered data, it was discovered that there is a direct relationship between the reactor volume and the profit obtained, while there is an inverse relationship with the dilution coefficient.

Table 2. Results

Reactor ID	Dilution Coeff. (day^{-1})	Biomass Con. (kg/m^3)	Profit ($)
1*	Low	0.59	19.63
2	Mid-Low	0.57	16.92
3	Mid	0.55	14.76
4	Mid-High	0.54	12.99
5	High	0.46	9.99

Table 3. Reactor Configurations

Reactor ID	Volume (m^3)	Radius (m)	Height (m)
1*	12.50	1.13	3.104
2	11.11	1.04	3.250
3	10.00	1.26	1.980
4	9.10	1.04	2.640
5	8.33	1.05	2.420

Uncertainty in income and expense parameters arises due to the complex interaction of various factors, such as market conditions, competition levels, macroeconomic indicators, technological advances, political and legal factors, natural disasters, customer behavior, and management decisions. These factors affect business revenues and expenses, causing uncertainty.

To address the uncertainties in economic parameters, 150 data sets were randomly created using normal distributions with a standard deviation of parameter values of 5% and lower and upper limits of 10% actual parameter value. From these data sets, 15 were randomly selected according to the number of scenarios. This method was used to diversify uncertainties in business revenues and expenses and consider different scenarios (Acevedo & Pistikopoulos, 1998). It has been observed that when parameter values are widely distributed and follow a normal distribution, they tend to be close to each other. Therefore, based on the study requirements, creating only 15 scenarios is sufficient to represent an adequate sample size.

Figure 2 displays the simulation results for Reactor 1, which represents the optimal outcome, and the corresponding distribution. The chart visually presents the diversity of data sets obtained based on different economic scenarios and the impact of this diversity on reactor performance. This helps to understand how business decisions may change according to various scenarios and the impact of uncertainties on business performance.

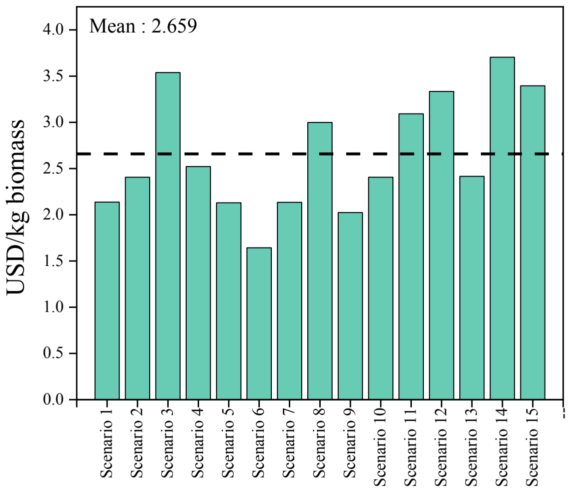

Figure 2. Profit Distribution of Scenarios.

The average profit was found to be 2.659 USD/kg of biomass. The 14th scenario yielded the highest profit (3.704 USD/kg of biomass), indicating positive conditions for the business and increased profitability. Conversely, the 6th scenario resulted in the lowest profit (1.643 USD/kg of biomass), suggesting a more challenging operating environment and decreased profitability. This evaluation emphasizes the importance of taking economic uncertainties and different scenarios into account when making strategic decisions for the business.

4. CONCLUSIONS

This study presents an updated MINLP model based on the traditional microalgae model. The model improves reactor selection, optimum reactor sizing, and achieving maximum biomass concentration by using five different dilution coefficients. A high-capacity reactor design was achieved by selecting low dilution coefficients, maximizing the amount of product as the optimum solution. In the dynamic MINLP model, economic parameters are included to maximize process profit. To introduce uncertainty into these variables, a normal distribution was used, resulting in a stochastic model. The results demonstrate the optimal reactor and operating conditions necessary to achieve maximum biomass concentration while considering operating costs and expenses.

In summary, the dynamic stochastic MINLP model provides effective and flexible solutions for complex decision-making problems. It allows decision-makers to adapt to changing parameters and uncertainties in real-world conditions. Furthermore, its stochastic structure contributes to risk management and improves optimization performance. This model can effectively be used in dynamic and uncertain environments, such as microalgae bioenergy production, to achieve cost-effectiveness and efficiency in industrial applications.

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