

T.R.
GEBZE TECHNICAL UNIVERSITY
GRADUATE SCHOOL

**STOCHASTIC AND MIXED INTEGER NONLINEAR
PROGRAMMING APPLICATIONS IN BIOCHEMICAL
PROCESSES**

SERCAN KIVANÇ

**A THESIS OF MASTER OF SCIENCE
DEPARTMENT OF CHEMICAL ENGINEERING**

ADVISOR: ASSOC. PROF DR. HASAN ŞILDIR

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GEBZE TEKNİK ÜNİVERSİTESİ
LİSANSÜSTÜ EĞİTİM ENSTİTÜSÜ

BİYOKİMYASAL PROSESLERDE STOKASTİK VE
KARMAŞIK TAM SAYILI DOĞRUSAL OLMAYAN
PROGRAMLAMA UYGULAMALARI

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ABSTRACT

In this thesis, a complex integer nonlinear programming model was developed to determine the optimum cultivation conditions by calculating the process variables that have a direct effect on the growth rate such as nutrient concentration, light color, dilution coefficient and feed stream purity in the production of biofuel and biomass from microalgae, one of the fourth generation renewable energy sources. In the model, maximum profitability and biomass density were calculated considering the physical and economic constraints. In the third part of the thesis, uncertainty was added to the economic parameters by modifying the developed mathematical model. This added uncertainty is very important in terms of testing the flexibility of the model against economic fluctuations and improving the decision-making ability of the model against variable cost/sales prices and calculating the optimum cultivation conditions.

In the fourth part of the thesis, unlike traditional photobioreactor models, the model equations were modified by using two independent variables (time and depth) in the model. Ordinary differential equations (ODE) in traditional models were replaced by partial differential algebraic equations. In this way, reactor modeling has been carried out in a more comprehensive and robust manner. In addition, unlike traditional modeling, uncertainty has been added to the model parameters, allowing the calculation of the maximum amount of biomass to be obtained in various scenarios. Thanks to the uncertainty added to the model parameters, the capacity to produce flexible and robust outputs under variable process conditions has been increased.

In the last part of the thesis, a mathematical model that includes the 24-hour short-term production planning of a large-scale production facility has been developed. This developed model offers a highly innovative structure thanks to its ability to simultaneously implement superstructure optimization and stochastic optimization concepts. In the case studies conducted within this scope, block and continuous production plans that minimize production costs were developed in the deterministic solution; and more flexible and adaptable production strategies were created by considering the uncertainties in the cost parameters in the stochastic solution. Finally, in the third case study, the effects of the number of event points used on model performance and solution results were analyzed in detail.

Keywords: Mixed Integer Nonlinear Programming (MINLP), Stochastic Optimization, Superstructure Optimization, Short Term Scheduling.

ÖZET

Bu tez çalışmasında kapsamında, dördüncü nesil yenilenebilir enerji kaynaklarından biri olan mikroalglerden biyoyakıt ve biyokütle üretiminde besi ortam konsantrasyonu, ışık rengi, seyreltme katsayısı ve besleme akımı saflığı gibi büyüme hızı üzerinde doğrudan etkiye sahip olan proses değişkenlerinin hesaplanarak optimum yetiştirme koşullarının belirlenmesine yönelik bir karmaşık tam sayılı doğrusal olmayan programlama modeli geliştirilmiştir. Modelde, fiziksel ve ekonomik kısıtlar göz önünde bulundurularak maksimum karlılık ve biyokütle yoğunluğu hesaplanması sağlanmıştır. Tezin üçüncü bölümünde, geliştirilen matematiksel modelde modifikasyon yapılarak ekonomik parametrelere belirsizlik eklenmiştir. Eklenen bu belirsizlik modelin ekonomik dalgalanmalara karşı esnekliğinin test edilmesi ve değişken maaliyet/satış fiyatları karşısında modelin karar verme yeteneğinin geliştirilmesi ve optimum yetiştirme koşullarının hesaplanabilmesi adına oldukça önemlidir.

Tezin dördüncü bölümünde, geleneksel foto biyoreaktör modellemelerinin aksine modelde iki bağımsız değişken (zaman ve derinlik) kullanılarak model denklemleri modifiye edilmiştir. Geleneksel modellerinde yer alan adi diferansiyel denklemler(ODE) yerlerini kısmi diferansiyel cebirsel denklemlere bırakmıştır. Bu sayede reaktör modellemesi daha kapsamlı ve sağlam bir şekilde gerçekleştirilmiştir. Ayrıca geleneksel modellemelerden farklı olarak, model parametrelerine belirsizlik eklenmiş olup bu sayede çeşitli senaryolarda elde edilecek maksimum biyokütle miktarının hesaplanmasına olanak tanınmıştır. Model parametrelerine eklenen belirsizlik sayesinde, değişken proses koşulları altında esnek ve sağlam çıktılar üretme kapasitesi arttırılmıştır.

Tezin son bölümünde ise, büyük ölçekte üretim yapan bir üretim tesisinin 24 saatlik kısa vadede üretim planlamasını içeren bir matematiksel model geliştirilmiştir. Geliştirilen bu model, üstyapı optimizasyonu ve stokastik optimizasyon konseptlerinin aynı anda gerçekleştirebilme yeteneği sayesinde oldukça yenilikçi bir yapı sunmaktadır. Bu kapsamda yürütülen vaka çalışmalarında, deterministik çözümde üretim maliyetini minimize eden blok ve sürekli üretim planları geliştirilmiş; stokastik çözümde ise maliyet parametrelerindeki belirsizlikler göz önünde bulundurularak daha esnek ve uyarlanabilir üretim stratejileri oluşturulmuştur. Son olarak, gerçekleştirilen üçüncü vaka çalışmasında, kullanılan olay noktası sayısının model performansı ve çözüm sonuçları üzerindeki etkileri detaylı biçimde analiz edilmiştir.

Anahtar Kelimeler: Karma Tam Sayılı Doğrusal Olmayan Programlama (MINLP), Stokastik Optimizasyon, Üstyapı Optimizasyonu, Kısa Vadeli Planlama.

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TABLE OF CONTENTS

	<u>Page</u>
ABSTRACT	v
ÖZET	vi
ACKNOWLEDGEMENTS	vii
TABLE OF CONTENTS	viii
LIST OF SYMBOLS AND ABBREVIATIONS	x
LIST OF FIGURES	xiv
LIST OF TABLES	xv
1. INTRODUCTION	1
2. SYNTHESIS of NANNOCOLOROPSIS OCULATA CULTIVATION PROCESS BASED on MIXED-INTEGER FORMULATIONS	3
2.1. Introduction	3
2.2. Model Development	7
2.2.1. Microalgae Growth Rate Models	7
2.2.2. Mass Balance Equations	9
2.2.3. Parameter Estimation	10
2.3. Case Studies	13
2.3.1. Case 1: Profit Maximization	15
2.3.2. Case 2: Biomass Concentration Maximization	20
2.3.3. Case 3: Biomass Concentration Maximization Under Variable Initial Concentration	22
2.3.4. Comparison of Case Studies	24
2.4. Conclusion	26
3. A MIXED-INTEGER DYNAMIC AND STOCHASTIC ALGAE PROCESS OPTIMIZATION	28
3.1. Introduction	28
3.2. Methodology	30
3.3. Results	33
3.4. Conclusion	36
4. DYNAMIC AND STOCHASTIC OPTIMIZATION of ALGAE CULTIVATION PROCESS	37
4.1. Introduction	37
4.2. Methodology	41
4.2.1. Spatiotemporal Model for Algae Bioreactor	41
4.2.2. Dynamic Formulation and Deterministic Optimization	46
4.2.3. Stochastic Optimization with Scenario Analysis	48
4.3. Results	50
4.3.1. Deterministic Optimization	51
4.3.2. Stochastic Optimization	53
4.3.2.1. Stochastic Optimization Based on Likely Parameter Range	53
4.3.2.2. Stochastic Optimization Based on Unlikely Parameter Range	57

4.4. Conclusion	60
5. INTEGRATED STOCHASTIC SCHEDULING AND SUPERSTRUCTURE OPTIMIZATION FOR SHORT TERM PRODUCTION PLANING	62
5.1. Introduction	62
5.2. Model Formulation	66
5.2.1. Allocation Constraint	66
5.2.2. Capacity Constraint	66
5.2.3. Stream Capacity Constraint	67
5.2.4. Material Balance Constraint	67
5.2.5. Duration Constraint	68
5.2.6. Sequence Constraint (Same Task in Same Unit)	69
5.2.7. Sequence Constraint (Different Task in Different Unit)	69
5.2.8. Sequence Constraint (Completion of Previous Tasks)	70
5.2.9. Time Horizon Constraint	70
5.2.10. Minimum Amount of Product	70
5.2.11. Mixer Cost Estimation	71
5.2.12. Reactor Cost Estimation	71
5.2.13. Separator Cost Estimation	72
5.2.14. Selection Constraints	72
5.2.15. Objective Function	72
5.3. Results	74
5.3.1. Case 1: Stochastic Scheduling	74
5.3.2. Case 2: Deterministic Scheduling	78
5.3.3. Case 3: Event Point Number	81
5.4. Conclusion	85
6. CONCLUSION	87
REFERENCES	89
BIOGRAPHY	98
PUBLICATIONS AND PRESENTATIONS FROM THESIS	99

LIST OF SYMBOLS AND ABBREVIATIONS

E	: Expenses (\$)
R	: Revenues (\$)
$X(t)$	: Biomass Concentration at time “ t ” (kg/m ³)
b_i	: Binary Variable for Selection of Photobioreactor (PBR) “ i ”
$V_{r,m}$	: Volume of Each Reactor “ m ” (m ³)
p_{fuel}	: Fuel Sales Price (\$/kg fuel)
$fuel_f$	: Fuel Sales Factor (kg fuel/kg-dry biomass)
p_{fert}	: Fertilizer Sales Price (\$/kg fertilizer)
$fert_f$	: Fertilizer Sales Factor (kg fertilizer/kg-dry biomass)
$p_{oper.costs}$	: Operating Costs (\$/kg-dry biomass)
$b_{med,q}$	: Binary Variables for Selection of Cultivation Medium “ q ”
p_{med}	: Cultivation Medium Price (\$/kg-dry biomass)
p_{water}	: Water Price (\$/m ³)
$\mu_x(t)$	: Specific Growth Rate at time “ t ” (1/days)
μ^{max}	: Maximum Specific Growth Rate (1/days)
ϕ	: Light Factor
α	: Weighting Factor
$\mu_N(t)$	: Maximum Specific Growth Rate in Nitrogen Limited Cultivation System (1/days)
β	: Weighting Factor
$\mu_P(t)$	: Maximum Specific Growth Rate in Phosphorus Limited Cultivation System (1/days)
δ	: Weighting Factor
$\mu_C(t)$	: Maximum Specific Growth Rate in Carbon Limited Cultivation System (1/days)
k_N	: Limiting Cell Quota of Nitrogen (kgN/m ³)
$N(t)$	: Nitrogen Concentration at time “ t ” (kg/m ³)
φ_N	: Utilization of Yield Coefficient of Nitrogen (kgX/kgN)
$b_{dr,m}$	: Binary Variable for Selection of Dilution Rate Coefficient and Reactor Size Pair “ m ”
D_m	: Dilution Rate Coefficient “ m ” (1/days)
k_P	: Limiting Cell Quota of Phosphorus (kgP/m ³)
$P(t)$	: Phosphorus Concentration at time “ t ” (kg/m ³)
φ_P	: Utilization of Yield Coefficient of Phosphorus (kgX/kgP)
k_l	: Overall Mass Transfer Coefficient (meter/days)
a	: Cell Surface Area (1/meter)
$CO_2(t)$	: Carbon Dioxide Concentration in Liquid Phase at time “ t ” (kg/m ³)
$C_x(t)$	: Free Carbon Dioxide Concentration in Cultivation Medium (kg/m ³)
k_C	: Limiting Cell Quota of Carbon (kgCO ₂ /m ³)
φ_{co2}	: Utilization Yield Coefficient of Carbon Dioxide (kgX/kgCO ₂)

$b_{col,j}$	: Binary Variables for Selection of Cultivation Light Color “j”
$\tau_{col,j}$	: Cultivation Efficiency with Light Color “j”
$b_{feed,k}$	: Binary Variables for Selection of Feed Stream “k”
$\omega_{feed,k}$	: Cultivation Efficiency with Feed Stream “k”
$b_{med,q}$	: Binary Variables for Selection of Cultivation Medium “q”
$\mu_{i,q}^{max}$	: Maximum Specific Growth Rate in Cultivation Medium “q” (1/days)
F_m	: Feed Flow Rate (m ³ /days)
$X(0)$	: Initial Biomass Concentration (kg/m ³)
$N(0)$	: Initial Nitrogen Concentration (kg/m ³)
$P(0)$	: Initial Phosphorus Concentration (kg/m ³)
$CO_2(0)$	: Initial Carbon Dioxide Concentration in Liquid Phase (kg/m ³)
γ	: Tuning Parameter for CO ₂ Balance
ST	: Total Scenario Number
$V_{r,i}$	: Volume of Reactor “i”
$X(t_f)$	: Biomass Concentration at final time
p_f	: Fuel Sales Price (\$/kg fuel)
f_f	: Fuel Sales Factor (kg fuel/kg-dry biomass)
p_{fr}	: Fertilizer Sales Price (\$/kg fertilizer)
f_{fr}	: Fertilizer Sales Factor (kg fertilizer/kg-dry biomass)
p_{oc}	: Operation Costs (\$/kg dry biomass)
p_w	: Water Price (\$/m ³)
$r_{i,min}$	: Minimum Radius of Reactor “i”.
r_i	: Radius of Reactor “i”
$r_{i,max}$	: Maximum Radius of Reactor “i”.
$h_{i,min}$	: Length Radius of Reactor “i”.
h_i	: Length of Reactor “i”
$h_{i,max}$	: Length Radius of Reactor “i”.
$f_x(S)$	: Function Expressing the Effect of Substrate Concentration on the Biomass Growth Rate.
$f_x(N)$	: Function Expressing the Effect of Nitrogen Concentration on the Biomass Growth Rate.
$f_x(I)$	: Function Expressing the Effect of Light Intensity Concentration on the Biomass Growth Rate.
$f_L(S)$	: Function Expressing the Effect of Substrate Concentration on the Lipid Growth Rate.
$f_L(N)$	: Function Expressing the Effect of Nitrogen Concentration on the Lipid Growth Rate.
$f_L(I)$	: Function Expressing the Effect of Light Intensity Concentration on the Lipid Growth Rate.
Y_S^X	: Yield Coefficient for Oil-Free Biomass Production with respect to the Substrate (gX/gS).
Y_S^L	: Yield Coefficient for Lipid Production with respect to the Substrate (gL/gS).

Y_N^X	: Yield Coefficient for Oil-Free Biomass Production with respect to the Nitrogen (gX/gN).
k_1	: Constant for Light Intensity (m^{-1})
k_2	: Constant for Light Intensity ($L \cdot \mu mole / g \cdot m^3 \cdot s$)
K_{XS}	: Substrate Saturation Coefficient for Biomass (gS/L).
K_{iXS}	: Substrate Inhibition Coefficient for Biomass (gS/L).
K_{XN}	: Nitrogen Saturation Coefficient for Biomass (gN/L).
K_{iXN}	: Nitrogen Inhibition Coefficient for Biomass (gN/L).
$q_{L,max}$	: Maximum Lipid Growth Rate (h^{-1}).
K_{LS}	: Substrate Saturation Constant for Lipid (gS/L)
K_{iLS}	: Substrate Inhibition Coefficient for Lipid (gS/L)
K_{iNL}	: Nitrogen Inhibition Coefficient for Lipid (gN/L)
K_I	: Saturation Coefficient for Lipid and Biomass Accumulation ($\mu mole / m^2 s$)
K_{il}	: Coefficient of Inhibition for Lipid and Biomass Deposition ($\mu mole / m^2 s$)
$L(t, x)$	: Lipid Concentration at time “t” and depth “x”.
$X(t, x)$	: Biomass Concentration (gS/L) at time “t” and depth “x”.
$\mu_x(t, x)$	: Biomass Accumulation (growth) Rate (h^{-1}) at time “t” and depth “x”.
$\mu_L(t, x)$	: Lipid Accumulation (growth) Rate (h^{-1}) at time “t” and depth “x”.
$S(t, x)$	: Substrate Concentration (gS/L) at time “t” and depth “x”.
$N(t, x)$	: Nitrogen Concentration (gS/L) at time “t” and depth “x”.
$I(t, x)$	: Light Intensity ($\mu mole / m^2 s$) at time “t” and depth “x”.
$\mu_{x,max}$	: Maximum Biomass Growth Rate (h^{-1}).
$q_{L,max}$	: Maximum Lipid Accumulation Rate (h^{-1}).
$y_{m,L,0}$	: Lower Bound for Variable “m” at Initial Time.
$y_{m,U,0}$	: Upper Bound for Variable “m” at Initial Time.
LBR_L	: Low Lipid/Biomass Ratio.
LBR_H	: High Lipid/Biomass Ratio.
$wv(i, n)$	: Binary Variables that Assign the Beginning of Task “i” at Event Point “n”.
$yv(j, n)$	: Binary Variables that Assign the Utilization of Unit “j” at event point “n”.
V_{ij}^{min}	: Minimum Amount of Material Processed by Task “i” Required to Start Operating Unit “j”.
b_j	: Equipment Selection Binary Variable of unit “j”.
$B(i, j, n)$	: Amount of Material Undertaking Task “i” in Unit “j” at Event Point “n”.
V_{ij}^{max}	: Maximum Amount of Material Processed by Task “i” Required to Start Operating Unit “j”.
$ST(s, n)$	: Amount of State “s” at Event Point “n”.
$ST(s)^{max}$	: Available Maximum Storage Capacity for State “s”.
$d(s, n)$	: Amount of State “s” Being Delivered to the Market at Event Point “n”.
ρ_{si}^p	: Proportion of state “s” Produced from task “i”
ρ_{si}^c	: Proportion of state “s” Consumed from task “i”

$T^f(i, j, n)$	: Time that Task “ i ” Finishes in Unit “ j ” While It Starts at Event Point “ n ”.
$T^s(i, j, n)$	: Time that Task “ i ” Starts in Unit “ j ” at Event Point “ n ”.
α_{ij}	: Constant Term of Processing Time of Task “ i ” at Unit “ j ”.
β_{ij}	: Variable Term of Processing Time of Task “ i ” at Unit “ j ” Expressing the Time Required by the Unit to Process One Unit of Material Performing Task “ i ”.
H	: Time Horizon.
J_i	: Set of Units which are Suitable for Performing Task “ i ”.
J	: Set of Process Units.
I	: Set of Overall Tasks.
I_j	: Tasks which can be Performed in Unit “ j ”.
S	: Set of all involved states “ s ”.
N	: Event Points within the Time Horizon.
Sc	: Set of Scenarios.
i	: Index of Tasks.
j	: Index of Units.
n	: Index of Event Points.
s	: Index of States.
sc	: Index of Scenarios
$C^{mix}(j, sc)$	: Cost of Mixer “ j ” in Scenario “ sc ” (\$).
$p_{m,cons}(1, j, sc)$	: Construction Cost of Mixer “ j ” in Scenario “ sc ” (\$/kg.h).
$p_{m,maint}(1, j, sc)$	: Maintenance Cost of Mixer “ j ” in Scenario “ sc ” (\$/kg.h).
$p_{m,energy}(1, j, sc)$	: Energy Cost of Mixer “ j ” in Scenario “ sc ” (\$/kg.h).
$p_{m,eff}(1, j, sc)$	: Efficiency of Mixer “ j ” in Scenario “ sc ”.
$C^{reac}(j, sc)$	: Cost of Reactor “ j ” in Scenario “ sc ” (\$).
$p_{r,lab}(2, j, sc)$	: Labor Cost of Reactor “ j ” in Scenario “ sc ” (\$/kg.h).
$p_{r,cons}(2, j, sc)$	: Construction Cost of Reactor “ j ” in Scenario “ sc ” (\$/kg.h).
$p_{r,fuel}(2, j, sc)$	: Fuel Cost of Reactor “ j ” in Scenario “ sc ” (\$/kg.h).
$p_{r,cat}(2, j, sc)$	: Catalyst Cost of Reactor “ j ” in Scenario “ sc ” (\$/kg.h).
$p_{r,util}(2, j, sc)$	: Utility Cost of Reactor “ j ” in Scenario “ sc ” (\$/kg.h).
$C^{sep}(j, sc)$	: Cost of Separator “ j ” in Scenario “ sc ” (\$).
$p_{s,solvent}(3, j, sc)$	: Solvent Cost of Separator “ j ” in Scenario “ sc ” (\$/kg.h).
$p_{s,constr}(3, j, sc)$	: Construction Cost of Separator “ j ” in Scenario “ sc ” (\$/kg.h).
$p_{r,utility}(3, j, sc)$	: Utility Cost of Separator “ j ” in Scenario “ sc ” (\$/kg.h).
$p_{s,eff}(3, j, sc)$	: Efficiency of Separator “ j ” in Scenario “ sc ”.
MINLP	: Mixed Integer Non-Linear Programming.
NLP	: Non-Linear Optimization
MILP	: Mixed Integer Linear Programming
MIQCP	: Mixed Integer Quadratic Constrained Programming
DAE	: Differential Algebraic Equation
PDAE	: Partial Differential Algebraic Equation
ODE	: Ordinary Differential Equation
BONMIN	: Basic Open-source Nonlinear Mixed Integer Programming
STS	: Short Term Scheduling

LIST OF FIGURES

	<u>Page</u>
Figure 2.1: Simplified mixed integer problem architecture.	14
Figure 2.2: Concentration profile for case 1.	18
Figure 2.3: Concentration profile for case 2.	21
Figure 2.4: Concentration profile for case 3.	24
Figure 2.5: Biomass concentration profile for all cases.	25
Figure 3.1: Concentration profiles of nutrients and biomass.	33
Figure 3.2: Profits of scenarios.	35
Figure 4.1: Scenario generation for stochastic model.	49
Figure 4.2: Spatial and temporal distribution of some variables a. lipid concentration profile b. light intensity profile.	52
Figure 4.3: Dynamic profile of compounds.	52
Figure 4.4: Light intensity histograms for likely scenarios a. LBR _L b. LBR _H .	54
Figure 4.5: Biomass concentration profiles in likely scenarios and x = 0.1 b. LBR _L and x = 0.9. c. LBR _H and x = 0.1. d. LBR _H and x = 0.9.	55
Figure 4.6: Lipid concentration profiles in likely scenarios. a. LBR _L and x = 0.1 b. LBR _L and x = 0.9. c. LBR _H and x = 0.1. d. LBR _H and x = 0.9.	56
Figure 4.7: Light Intensity Histograms for Unlikely Scenarios a. LBR _L b. LBR _H .	58
Figure 4.8: Biomass concentration profiles in unlikely scenarios a. LBR _L and x = 0.1 b. LBR _L and x = 0.9. c. LBR _H and x = 0.1. d. LBR _H and x = 0.9.	58
Figure 4.9: Lipid concentration profiles in unlikely scenarios a. LBR _L and x = 0.1 b. LBR _L and x = 0.9. c. LBR _H and x = 0.1. d. LBR _H and x = 0.9.	59
Figure 5.1: Superstructure of the problem.	73
Figure 5.2: Parameter generation with $\mu = 1$ and $\sigma = \pm 0.5$.	74
Figure 5.3: Results of stochastic model.	76
Figure 5.4: STS results for deterministic model.	79
Figure 5.5: Cost / tone for each event point simulation.	82
Figure 5.6: STS results for a. 7 event point b. 8 event point c. 9 event point d. 10 event point	84

LIST OF TABLES

	<u>Page</u>
Table 2.1: Results of the parameter estimation.	13
Table 2.2: Number of variables and constraints in case studies.	15
Table 2.3: Cost and sale prices.	17
Table 2.4: Results for case 1.	18
Table 2.5: Scenarios at different design variables.	20
Table 2.6: Results of case 2.	22
Table 2.7: Summary of case studies.	24
Table 3.1: Growth parameter values.	33
Table 3.2: Result of simulations	34
Table 3.3: Continuation of results.	34
Table 4.1: Reaction kinetic models.	42
Table 4.2: Light intensity distribution expressions.	43
Table 4.3: Parameter values defining the photobioreactor model.	46
Table 4.4: Deterministic optimization results.	51
Table 4.5: Results of likely case studies.	53
Table 4.6: Results of likely case studies (continue).	54
Table 4.7: Results of unlikely case studies.	57
Table 5.1: Cost distribution for each scenario.	75
Table 5.2: Cost distribution for each process unit.	79
Table 5.3: Results for each event point.	81

1. INTRODUCTION

The rapidly increasing world population, along with developing industrialization and technology, necessitates the development of sustainable systems that aim to minimize environmental impacts in all production sectors while maintaining efficiency and product quality at the highest level. In this context, the role of renewable energy sources is of great importance in ensuring environmental sustainability. In particular, microalgae-based biomass and biofuel production, which contributes to the reduction of carbon emissions, is a renewable energy solution that promises potential in terms of both environmental friendliness and economy. Microalgae, which can convert CO₂ into bioenergy through photosynthesis and various biochemical reactions, are an important biological resource for the development of sustainable energy systems.

Determining the optimum process conditions in biomass and biofuel production from microalgae is of critical importance in terms of efficient use of nutrients, increasing the CO₂ conversion rate and maximizing overall production efficiency. Although many experimental studies have been conducted in the literature for this purpose, it has become possible to achieve more systematic and generalizable results thanks to the integration of mathematical modeling into the process.

In this context, in the second part of the thesis, a series of simulation studies were carried out in order to determine the optimum cultivation conditions of microalgae of the species *Nannochloropsis Oculata* and to achieve production with maximum profitability. In the developed mathematical model; biomass production was optimized by considering parameters such as growth rate, medium component concentrations, light color, dilution coefficient, feed stream purity. With this model, optimum conditions were determined based on both biological efficiency and economic gain.

In the third part of the thesis, the flexibility of the model was increased by adding uncertainties to the cost parameters and the optimum dilution coefficient and reactor sizing were calculated under variable market conditions. Thus, the model was structured to produce reliable results not only under fixed conditions but also under economic variables.

In the fourth part, a partial differential algebraic equation (PDAE) based model was developed that represents more realistic system dynamics compared to previous models and includes time and location dependent variables. In this model, light intensity and nutrient distribution affecting microalgae growth were considered in two dimensions and simulations were performed with both deterministic and stochastic solution methods. Thus, more reliable predictions regarding system performance under different scenarios were provided by also considering parameter uncertainties

In the fifth section, an optimization model that performs 24-hour short-term production planning of production facilities was developed for the integration of macro-scale industrial production systems. This developed model, unlike traditional production planning approaches, includes both superstructure optimization and stochastic modeling in a holistic manner. This innovative approach offers flexible planning solutions that can adapt to variable market conditions, use resources effectively and support sustainable production.

In the last section, the main findings obtained in the study, the limitations of existing methods and the original contributions of the proposed models are summarized; evaluations and suggestions for further research are presented.

2. SYNTHESIS of *NANNOCHLOROPSIS OCULATA* CULTIVATION PROCESS BASED on MIXED-INTEGER FORMULATIONS

2.1. Introduction

The industrial revolution and the spread of large-scale manufacturing, along with the growth of the world's population, led to a significant increase in the use of fossil fuels to meet energy demand [1]. However, this increase has caused environmental problems due to the accumulation of harmful gases such as carbon dioxide (CO₂), methane (CH₄), nitrogen oxides (NO_x), and sulfur oxides (SO_x) in the atmosphere [2]. As part of efforts to solve these problems, various research and development activities have been carried out to favor the investment in renewable energy sources and energy efficiency for the design of low emission processes. In parallel, Carbon Capture, Utilization and Storage (CCUS) studies also have gained significant attention to processing the harmful gases once they are produced. The ultimate goal is to reduce the amount of CO₂, as considered the major pollutant for most cases, released into the atmosphere through geological storage, ocean storage, mineralization and biological processes, which are one of the storage methods [3], despite issues associated with long-term effectiveness, environmental impact, economic feasibility, and storage security [4], [5]. Photosynthesis is a biochemical conversion performed by certain types of algae and bacteria [6] to obtain oxygen and biomass by utilizing carbon dioxide and usually nitrate and phosphate-based nutrients from wastewater or other sources [7]–[11]. In this context, the microalgae species, with a promising lipid content, accounts for the significant fraction of the dry biomass at the end of the cultivation process [12]–[15]. The resulting lipid is converted to fatty acid methyl ester through a series of purification and transesterification reactions to obtain biodiesel. In addition, microalgae-based biomass can be used to produce nutraceuticals and dietary supplements, pharmaceuticals, cosmetics, animal feed, wastewater treatment, bioplastics, and fertilizers [16]. Thus, the development of formulations aimed at process synthesis and optimization to ensure large-scale production from microalgae-based biomass becomes an important focus.

Large-scale microalgae cultivation is generally divided into open and closed systems.

Open systems use cultivation ponds, typically 10-40 cm deep, which have the advantage of low investment and operating costs. However, their efficiency is compromised by a higher risk of contamination and increased sensitivity to temperature fluctuations and evaporation [17]. In contrast, closed systems, also known as photobioreactor systems, include tubular, columnar, and flat-plate reactors are operated under tightly controlled process conditions. In practice, microalgae cultivation is strongly influenced by many factors, including temperature, pH, nutrient concentration, CO₂ supply, light intensity, photobioreactor lighting, oxygen concentration, and reactor orientation [18]–[20]. Wise selection and manipulation of these factors are essential to ensure profitability and efficiency, sustainability, non-toxic and biodegradable fuel production, and conservation of waste resources to eliminate the issues from a wide spectrum including excessive exposure to direct light, temperature control problems, overpopulation, toxic effects of produced oxygen, contamination, and pH fluctuations [21], [22].

To overcome the challenges and exploit the potential benefits of microalgae cultivation, sophisticated modeling and optimization tasks are necessary. Bekirogullari et al. presents a kinetic model for microalgal cultivation that has been experimentally validated using *Chlamydomonas Reinhardtii* [23]. The model considers carbon/nitrogen concentration, light intensity, and temperature to optimize lipid productivity. The results show a 50.9% increase in lipid productivity compared to the base case, demonstrating the effectiveness of the model for designing and optimizing microalgal oil production. Talaghat et al. presents the models accurately predict the effects of varying temperature, catalyst concentration, and methanol to oil ratio, revealing direct relationships with biodiesel yield. The research demonstrates that achieving over 99% efficiency in biodiesel production from microalgae is possible under optimal conditions [24]. Jayaraman et al. optimizes the microalgae biomass growth for renewable biofuels using stochastic programming which considers natural variability and day-to-night solar energy fluctuations and using multiplayer direct search. The results demonstrate that accounting for such fluctuations significantly improves profitability [25].

Azari et al. optimized biofuel production from *Chlorella Vulgaris* by introducing various impacts such as temperature, light, carbon concentration, aeration rate, pH, and time. The optimum conditions for biofuel production were calculated using

Genetic Programming, and were found to be 26°C temperature, 3200 lx light, 6% CO₂ concentration, and an aeration rate of 0.5 vvm over 11 days [26]. Galanopoulos et al. presents a superstructure framework for optimizing an integrated algae biorefinery using AIMMS to minimize biodiesel production costs by integrating wastewater and CO₂ emissions from a wheat straw biorefinery. The superstructure comprises seven stages, including cultivation identified as the most expensive stage. Their approach delivers up to 80% reduction in biodiesel production costs, demonstrating the economic benefits of the integrated concept over a standalone algae biorefinery [27]. Gong et al. present a new superstructure of an algal biorefinery for carbon sequestration and utilization. The problem is a mixed-integer nonlinear programming (MINLP), from which an open cultivation system is selected to reduce the unit cost of carbon. The ultimate design ensures the complete utilization of CO₂, resulting in zero direct emissions [28].

Wu et al. present a method for producing diesel and ethanol simultaneously from microalgae with estimated break-even prices of \$0.49/kg and \$2.61/kg, respectively, and an internal rate of return of 29.21% [29]. Béchet et al. presents a dynamic control strategy for optimizing the productivity of algal raceway ponds while minimizing their environmental impact. The strategy involves adjusting pond depth and retention time based on seasonal changes. Simulations conducted in various climates demonstrate that this approach can increase productivity by 0.6-9.9% and reduce water demand by 10-61%, thereby significantly decreasing the water footprint. Locally optimized dynamic process control is crucial when evaluating the feasibility of algae cultivation, as evidenced by the significant impact on algal productivity resulting from a strategy tailored to local conditions [30]. Hurst et al. presents a modified algae growth model in a raceway pond with variable depth, which includes a state variable and control for variable outflow. By utilizing numerical optimal control methods, the study demonstrates a significant 67% increase in lipid yield compared to a fixed pond depth [31].

Figuerola-Torres et al. presents a multi-parameter kinetic model for microalgal growth, starch, and lipid formation under nitrogen-limited mixotrophic conditions. The model is based on rigorous laboratory experiments with *Chlamydomonas Reinhardtii* and validated against various datasets. Using optimal nutrient-based cultivation strategies leads to a significant increase in starch and lipid production compared to the base-case

conditions [32]. De-Luca et al. optimizes microalgae-based processes by addressing the impact of inaccurate weather forecasts during cultivation. Two optimization approaches prevent critical conditions, such as cell death due to high temperatures, ensuring reliability in terms of productivity loss and water demand [33].

Unlike traditional optimization approaches, few studies have tackled the simultaneous synthesis and optimization problem for such problems while considering dynamic transitions under well-defined process-related constraints. MINLPs appear in many engineering branches with their capability to address both design operational tasks and thus applied in various fields, such as production planning, logistics, energy systems, finance, and biochemical processes, demonstrating their versatility and effectiveness [34]–[38].

Previously, Kivanc et al. presented stochastic optimization of *Nannochloropsis Oculata* algae growth under economic uncertainty to maximize profit. However, the study lacks the parameter estimation issues and does not cover high number of process design variables which have high significance in industrial process development, resulting an easy-to-solve optimization problem, relatively, and focuses on the selection of dilution coefficient explicitly only. On the other hand, the model conclusions become more realistic once a higher number of design variables and operational concerns are met in a comprehensive and simultaneous optimization problem for various objective functions under different process related constraints, which might require different superstructural modifications to be operated at different regimes and deliver significant superiority considering the engineering requirements [39].

This study focuses on the development of an MINLP to address the selection of major design variables and calculation of optimum operation conditions under dynamic considerations tightened by process related constraints. The design variables are introduced through binary variables to account for convenient selection of growth medium, light colour, feed stream impurity, reactor size and dilution coefficient in addition to several decision variables with continuous nature to employ different objective functions. Those advancements are implemented mainly on the model provided by Tijani et al., on which parameter estimation through nonlinear programming for advanced and subsequent computations are performed, as well, on a complex differential algebraic set of equations [40]. Next, the model expressions are

further processed to obtain MINLP for the calculation of design and operational variables, in addition to model architecture related intermediate variables, in a simultaneous fashion through Python/Pyomo environment to enable interface to different rigorous optimization algorithms, when needed. Although the resulting formulation suffers from a nonconvex formulation, and cannot address the global optimality concerns, the three case studies which are solved through local approach have demonstrated the conflicting design variable decision based on commonly used objective functions, including profit and biomass maximization. Furthermore, the formulation shows the contribution of increased degree of freedom to address the ultimate harness.

2.2. Model Development

2.2.1. Microalgae Growth Rate Models

Microalgae growth rates can be described by employing three common kinetic models: Monod, Haldane, and Droop. The Monod kinetic model includes the impact of individual nutrients on the growth rate of microalgae through a relatively simpler formulation to represent algal growth rates and given by [41]:

$$\mu = \mu^{max} \frac{S}{K_s + S} \quad (2.1)$$

where μ^{max} is the maximum specific growth; K_s is the saturation coefficient; and S is the substance concentration. Despite computational superiority with a relatively simple formulation, applicability is limited at high substrate concentrations where the maximum growth rate and substrate concentration are independent. Additionally, this model does not account for the inhibitory effects of toxic substances present in the substrate, makes it improper for such cases, as well. Furthermore, the Monod model does not incorporate the kinetics, lag, and death phases of the growth curve [42].

The Haldane model introduces the inhibition constant, K_i , to the Eq. 2.2. for the inhibitory effect, increasing the applicability, is expressed as:

$$\mu = \mu^{max} \frac{S}{K_s + S + \frac{S^2}{K_i}} \quad (2.2)$$

The Droop model is based on a cell quota-based approach for measuring nutrient levels in cells and applicable to unsteady state modelling, as well. Although the Droop model has a better representative capability, implementations are more scarce in the literature due to measurement difficulties and limitations [41].

$$\mu = \mu^{max} \left(1 - \frac{Q_{min}}{Q}\right) \quad (2.3)$$

where Q_{min} is the minimum cell quota; and Q is the quota. Following equation is introduced to represent the impacts of nitrogen, phosphorus, and carbon dioxide concentrations on the growth rate [40]:

$$\mu_x(t) = \mu^{max} \cdot [(\alpha \cdot \mu_N(t)) + (\beta \cdot \mu_P(t)) + (\delta \cdot \mu_C(t))] \cdot \phi \quad (2.4a)$$

where;

$$\mu_N(t) = \left[1 - \frac{k_N}{[N(t)]}\right] \frac{[X(t)]}{\gamma_N} - \frac{D}{\mu^{max}} [N(t)] \quad (2.4b)$$

$$\mu_P(t) = \left[1 - \frac{k_P}{[P(t)]}\right] \frac{[X(t)]}{\gamma_P} - \frac{D}{\mu^{max}} [P(t)] \quad (2.4c)$$

$$\mu_C(t) = k_l \cdot a \cdot \frac{[CO_2(t)](1 - D) - [C_x(t)]}{\mu^{max}} - \left[1 - \frac{k_{CO_2}}{[CO_2(t)]}\right] \frac{[X(t)]}{\gamma_{CO_2}} \quad (2.4d)$$

where 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 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); $k_l \cdot a$ coefficient was limited to the range of 107-156 d⁻¹ based on the experimental data by Tijani et al. [40]. α , β and δ are weighting factors and are 0.197, 0.079 and 0.441, respectively. 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. Tijani et al. provided the ϕ is in the range of 0.58-0.91 [40]. D represents the dilution coefficient and is obtained from:

$$D = \frac{F}{V} \quad (2.5)$$

where F is volumetric flow rate, and V is the reactor volume.

2.2.2. Mass Balance Equations

Time dependent ODEs of biomass, nitrogen (N), phosphorus (P), and carbon dioxide (CO₂) are specified below, mostly relying on the study of [40]:

$$\frac{dX}{dt} = \mu_X \cdot [X(t)] - D \cdot [X(t)] \quad (2.6a)$$

$$\frac{dN}{dt} = -\mu_X \frac{[X(t)]}{\gamma_N} - D \cdot [N(t)] \quad (2.6b)$$

$$\frac{dP}{dt} = -\mu_X \frac{[X(t)]}{\gamma_p} - D \cdot [P(t)] \quad (2.6c)$$

$$\frac{dCO_2}{dt} = \varphi \frac{dX}{dt} \quad (2.6d)$$

$$\frac{dC_x}{dt} = 0 \quad (2.6e)$$

where φ represents tuning parameter for CO₂ uptake to biomass from the environment. In the current study, the carbon dioxide mass balance equations were modified, compared to the reference study, to obtain a more simplified model that allows for more sophisticated optimization problem solutions due to its linear and computationally more favorable nature [40], [43]. However, such formulation would still deliver the patterns compatible with actual growth. Additionally, it is assumed that the level of CO₂ concentration in the cultivation medium remains constant due to the continuous feed of carbon dioxide. In the reference study [40], the unreacted carbon dioxide concentration was treated as a free variable.

2.2.3. Parameter Estimation

A typical nonlinear optimization problem (NLP) is defined by:

$$\min_x f(x) \quad (2.7a)$$

s. t.

$$g_i(x) \leq 0 \quad i = 1, \dots, m \quad (2.7b)$$

$$h_j(x) = 0 \quad j = 1, \dots, p \quad (2.7c)$$

where objective function is denoted by f ; x is the vector of decision variables; g and h are inequality and equality constraints, respectively.

Parameter estimation problem, through NLP, becomes more challenging once the data are collected from a dynamic regime, which is a typical case for micromicroalgae processes. The model for such processes are represented by Differential Algebraic Equations and defined by:

$$\frac{dx(t, \theta)}{dt} = f_{ODE}(t, x(t, \theta), \theta) \quad (2.8a)$$

$$y(x, \theta) = f_A(x(t, \theta), \theta) \quad (2.8b)$$

$$x(t_0) = x_0 \quad (2.8c)$$

where f_{ODE} and f_A are ODEs and algebraic equations, respectively; y is the measurable process variable; x_0 refers to the initial concentration of state variables; θ is the parameter vector to account for model related constants including pre-exponential factor, activation energy etc [34]. In the absence of direct measurement, parameter estimation based on model predictions and measured data allows the development of subsequent optimization problems with accuracy and reliability. For this purpose, the developed parameter estimation problem is as follows:

$$\min_{\theta} Q_{LS}(\theta) \quad (2.9a)$$

$$s. t. \quad (2.9b)$$

$$\theta_{min} \leq \theta \leq \theta_{max} \quad (2.9c)$$

$$\frac{dx(t, \theta)}{dt} = f(t, x(t, \theta), \theta) \quad (2.9d)$$

$$y(x, \theta) = g(x(t, \theta), \theta) \quad (2.9e)$$

$$x(t_0) = x_0, t \in [t_0, t_f] \quad (2.9f)$$

where θ_{min} and θ_{max} are the lower and upper bounds of the parameters, respectively; Q_{LS} is the weighted sum of squares of the residual and given by [34]:

$$Q_{LS} = \sum_{i=1}^n w_i (y_i(x, \theta) - \tilde{y}_i)^2 \quad (2.10)$$

where $\tilde{y}_i$ is the i^{th} measurement; w_i is the weighting parameter for corresponding data; n is the number of data. In this research, w_i is set to 1. Proposed model contains 13 parameters, out of three (α , β , and δ) were obtained from Tijani et al. [40]. The remaining parameters are estimated upon available measurements, as shown in Eq. 2.11., which include the concentrations of nitrogen, phosphorus, carbon dioxide and growth rates. Those measurements are collected at 2-day intervals throughout the 26-day experimental procedure and used as experimental data to estimate remaining 10 parameters:

$$\min_{\theta} (\tilde{\mu}_x - \mu_x(t))^2 + (\tilde{N} - N(t))^2 + (\tilde{P} - P(t))^2 + (\tilde{CO}_2 - CO_2(t))^2 \quad (2.11a)$$

$$s. t.$$

$$\mu_x(t) = \mu_{max} \cdot [(\alpha \cdot \mu_N) + (\beta \cdot \mu_P) + (\delta \cdot \mu_C)] \cdot \phi \quad (2.11b)$$

$$\mu_N(t) = [1 - \frac{k_N}{[N(t)]}] \cdot \frac{[X(t)]}{\gamma_N} - \frac{D}{\mu_{max}} \cdot [N(t)] \quad (2.11c)$$

$$\mu_P(t) = [1 - \frac{k_P}{[P(t)]}] \cdot \frac{[X(t)]}{\gamma_P} - \frac{D}{\mu_{max}} \cdot [P(t)] \quad (2.11d)$$

$$\mu_c(t) = k_l \cdot a \cdot \frac{[CO_2(t)] \cdot (1 - D) - [C_x(t)]}{\mu_{max}} - \left[1 - \frac{k_{CO_2}}{[CO_2(t)]}\right] \cdot \frac{[X(t)]}{\gamma_{CO_2}} \quad (2.11e)$$

$$\frac{dX}{dt} = \mu_x \cdot [X(t)] - D \cdot [X(t)] \quad (2.11f)$$

$$\frac{dN}{dt} = -\mu_x \cdot \frac{[X(t)]}{\varphi_N} - D \cdot [N(t)] \quad (2.11g)$$

$$\frac{dP}{dt} = -\mu_x \cdot \frac{[X(t)]}{\varphi_p} - D \cdot [P(t)] \quad (2.11i)$$

$$\frac{dCO_2}{dt} = \gamma \frac{dX}{dt} \quad (2.11h)$$

$$\frac{dC_x}{dt} = 0 \quad (2.11j)$$

$$\mu_{max} \geq \mu_x(t) \quad (2.11k)$$

$$\theta_{min} \leq \theta \leq \theta_{max} \quad (2.11l)$$

$$X(0) \geq X(0)_{min} \quad (2.11m)$$

$$N(0)_{min} \leq N(0) \leq N(0)_{max} \quad (2.11n)$$

$$P(0) \geq P(0)_{min} \quad (2.11o)$$

$$CO_2(0) \geq CO_2(0)_{min} \quad (2.11p)$$

where objective function includes growth rate, nutrients, and biomass measurements ($\tilde{\mu}_x, N, P, CO_2$). ODEs and algebraic equations are model related constraints and in turn deliver the predictions to perform comparison to actual measurements. In the formulation, lower and upper limits, θ_{min} and θ_{max} , are additionally assigned to the variables to tighten the search space based on the available physical knowledge during the optimization iterations. Furthermore, a constraint is added to the model to ensure that the maximum growth rate is equal to or greater than the growth rate at any time t . Lower and upper bounds are determined based on empirical data and graphs presented in the reference study [40].

Eq. 2.11a-p is solved using Python/Pyomo, an advanced programming language which provides interface to solvers of many complex problems including MINLPs [44]. Dynamic model expressions are discretized with predefined schemes. Interior Point Optimizer (IPOPT) is used for parameter estimation and the results are presented in **Table 2.1** [45].

Table 2.1: Results of the parameter estimation.

Parameter	Value	Unit	Parameter	Value	Unit
μ^{max}	0.31000	d ⁻¹	$k_l \cdot a$	127.519	d ⁻¹
k_N	0.02285	kgN/m ³	D	0.0999	d ⁻¹
φ_N	851.624	kgX/kgN	α	0.1970	--
k_P	0.00006	kgP/m ³	β	0.0790	--
φ_P	195.105	kgX/kgP	δ	0.4410	--
k_C	0.23680	kgCO ₂ /m ³	ϕ	0.8760	--
φ_{co2}	0.00923	kgX/kgCO ₂	γ	0.0980	--

2.3. Case Studies

In this section, we present several case studies to demonstrate the impact of simultaneous design and dynamic optimization of *Nannochloropsis Oculata* microalgae processes. The proposed formulations require significant theoretical background to exploit all available economic and process related improvements with simultaneous synthesis and operation considerations. The models developed in the case studies were mostly built upon the derivation and assumptions from Tijani et al.[40]. Additionally, further assumptions were incorporated to ensure the solvability of this model. These assumptions are as follows:

- The composition of the input material is deficient in microalgal inoculum, and the specific growth rate of the microalgae is correlated with four parametric input functions (nitrogen, phosphorus and carbon concentration as well as light intensity).
- It was assumed that light limitation for a continuous flow photobioreactor system could be used to describe the energy balance of the cultivation system, provided that

the incident light was fully photosynthetically harnessed.

- The effect of temperature and pH assume constant. 6
- The yield coefficients are fixed and remain constant.
- Free Carbon Dioxide Concentration remains constant due to the continuous supply.
- The self-shading effect (accumulation of microalgae) is ignored, and the light factor is considered constant regardless of the reactor location and biomass concentration.
- Dead Phase is not included in mathematical expressions.

The case studies include nonlinear and nonconvex expressions based on the complexity of the process dynamics, further tailored to include binary variables to represent the selection of design variables. The resulting MINLP formulations are solved to local optimum using BONMIN solver and simplified problem architecture is shown in **Figure 2.1**. Advanced reformulations and decomposition tasks are out of scope and left as future work to address global optimality and multiplicity concerns.

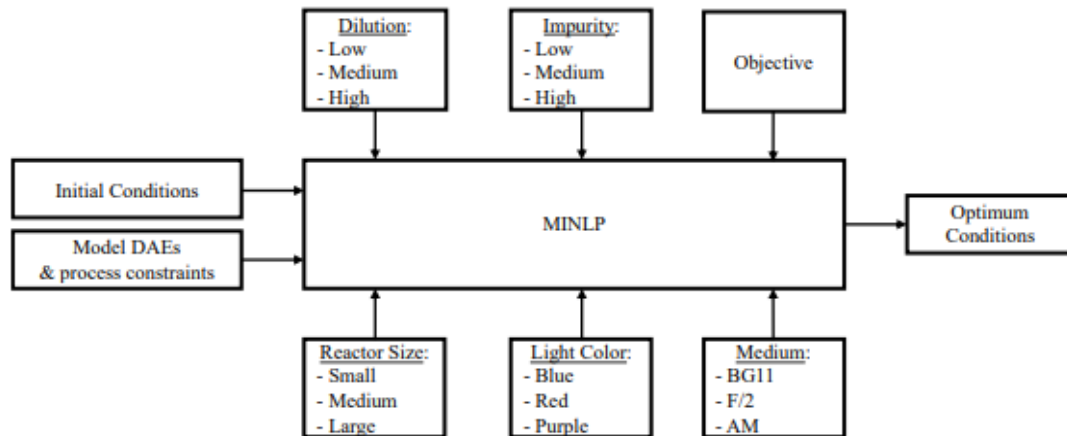


Figure 2.1: Simplified mixed integer problem architecture.

In addition to complexity of formulation complexity, there is a notable degree of freedom for the optimization problem whose size is presented in **Table 2.2**. Note that some of the constraints in **Table 2.2** are inactive box constraints on variables for programming purposes.

Table 2.2: Number of variables and constraints in case studies.

	Variables		Constraints	
	Continuous	Binary	Linear	Nonlinear
Dimension	594	15	329	270

2.3.1. Case 1: Profit Maximization

MINLP formulation to maximize the profit at the final time is given by:

$$\min_{X,P,N,CO_2,C_x,\mu_x,b_i,F_i} E - R \quad (2.12a)$$

$$R = X(t_f) \cdot \left(\sum_{i=1}^3 b_{reac,i} V_i \right) \cdot (p_{fuel} fuel_f + p_{fert} fert_f) \quad (2.12b)$$

$$E = X(t_f) \cdot \left(\sum_{i=1}^3 b_{reac,i} V_i \right) \cdot \left(\sum_{oper.costs} p_{oper.costs} + \sum_{q=1}^3 b_{med,q} p_{med} \right) + p_{water} \sum_{i=1}^3 b_{reac,i} V_i \quad (2.12c)$$

subject to:

$$\mu_x(t) = \mu^{max} \phi(\alpha \cdot \mu_N(t) + \beta \cdot \mu_P(t) + \delta \cdot \mu_C(t)) \quad (2.12d)$$

$$\mu_N(t) = \left(\left[1 - \frac{k_N}{[N(t)]} \right] \cdot \frac{[X(t)]}{\varphi_N} - \frac{\sum_{i=1}^3 (b_{dil,m} \cdot D_m)}{\mu^{max}} [N(t)] \right) \quad (2.12e)$$

$$\mu_P(t) = \left(\left[1 - \frac{k_P}{[P(t)]} \right] \cdot \frac{[X(t)]}{\varphi_P} - \frac{\sum_{i=1}^3 (b_{dil,m} \cdot D_m)}{\mu^{max}} [P(t)] \right) \quad (2.12f)$$

$$\mu_C(t) = k_l \cdot a \cdot [CO_2(t)] (1 - \sum_{i=1}^3 (b_{dil,m} \cdot D_m)) - [C_x(t)] - \left[1 - \frac{k_C}{[CO_2(t)]} \right] \cdot \frac{\mu^{max} [X(t)]}{\varphi_{co2}} \quad (2.12g)$$

$$\mu^{max} = \sum_{j=1}^3 \sum_{k=1}^3 \sum_{q=1}^3 b_{col,j} \tau_{col,j} b_{feed,k} \omega_{feed,k} b_{med,q} \mu_q^{max} \quad (2.12h)$$

$$\frac{dX}{dt} = \mu_X(t) \cdot [X(t)] - \sum_{m=1}^3 (b_{dil,m} \cdot D_m) \cdot [X(t)] \quad (2.12i)$$

$$\frac{dN}{dt} = -\mu_X(t) \cdot \frac{[X(t)]}{\varphi_N} - \sum_{m=1}^3 (b_{dil,m} \cdot D_m) \cdot [N(t)] \quad (2.12j)$$

$$\frac{dP}{dt} = -\mu_X(t) \cdot \frac{[X(t)]}{\varphi_p} - \sum_{i=1}^3 (b_{dil,m} \cdot D_m) \cdot [P(t)] \quad (2.12k)$$

$$\frac{dCO_2}{dt} = \gamma \frac{dX}{dt} \quad (2.12l)$$

$$\frac{dC_x}{dt} = 0 \quad (2.12m)$$

$$\sum_{i=1}^3 b_{reac,i} = \sum_{j=1}^3 b_{col,j} = \sum_{k=1}^3 b_{feed,k} = \sum_{m=1}^3 b_{dil,m} = \sum_{q=1}^3 b_{med,q} = 1 \quad (2.12n)$$

$$0 \leq X(t), 0 \leq N(t), 0 \leq P(t), 0.2 \leq CO_2(t), 0.25 \leq C_x(t) \quad (2.12o)$$

$$X(0) = 0.1000, N(0) = 0.2944, P(0) = 0.0591, CO_2(0) = 0.3805 \quad (2.12p)$$

where R is the revenue and calculated using fuel sales price, p_{fuel} ; $fuel_f$ is fuel sales factor; p_{fert} is fertilizer sales price; $fert_f$ is fertilizer sales factor; E is expense; $p_{oper.costs}$ is total operating cost and obtained from the summation of items in **Table 2.3**; p_{water} is water price; $b_{reac,i}$ is the binary variable for the selection of ; V_i is the reactor volume; $b_{feed,k}$ is binary variable for the feed impurity selection; $\omega_{feed,k}$ is a parameter relates the impurity level to growth rate which introduced by [46]; $b_{med,q}$ is binary and accounts for the selection of cultivation medium (f/2, BG11, and Algal Medium); $b_{col,j}$ represents the selection of a particular light color among red, purple, and blue; $\tau_{col,j}$ is a parameter and denotes the impact of light color on the maximum growth rate and obtained from [47]; μ_q^{max} represents the maximum biomass specific growth rate under corresponding cultivation medium based on [48] to account for the minerals affecting the growth; $X(0)$, $N(0)$, $P(0)$, and $CO_2(0)$ are initial concentrations of biomass, nitrogen, phosphorus and CO_2 , respectively. $fuel_f$ and $fert_f$ account for losses due to separation process after the reaction and assumes only 30% of the biomass is converted into fuel and fertilizer, respectively.

Eq. 2.12. is solved using the prices defined in **Table 2.3**:

Table 2.3: Cost and sales prices.

	Items	Value	Unit
Operating Costs	Initial Investment	0.39	\$/ (kg- dry biomass)
	Infrastructure	1.05	\$/ (kg- dry biomass)
	Fuel	0.48	\$/ (kg- dry biomass)
	Labor	3.18	\$/ (kg- dry biomass)
	Maintenance	3.10	\$/ (kg- dry biomass)
	Administration	0.75	\$/ (kg- dry biomass)
	Electricity	0.23	\$/ (kg- dry biomass)
	Water	0.30	\$/ (m ³)
Medium Cost	AM	0.15	\$/ (m ³)
	f/2	0.30	\$/ (m ³)
	BG11	0.80	\$/ (m ³)
Revenue	Fuel Sell Price	30.00	\$/kg fuel
	Fuel Sell Factor	0.30	(kg fuel/kg-dry biomass)
	Fertilizer Sell Price	5.00	\$/kg fertilizer
	Fertilizer Sell Factor	0.30	(kg fertilizer/kg-dry biomass)

Results of Case study 1 is given as follows:

Figure 2.2 includes the dynamic behavior of major process variables to represent algae growth. The lag phase, in which the microalgae inoculum added to the reactor medium does not show a significant increase in biomass as it acclimates to the new environment, is observed until day 2, approximately. The following 23-day periods indicate the exponential growth phase in which cells consume substrates and proliferate

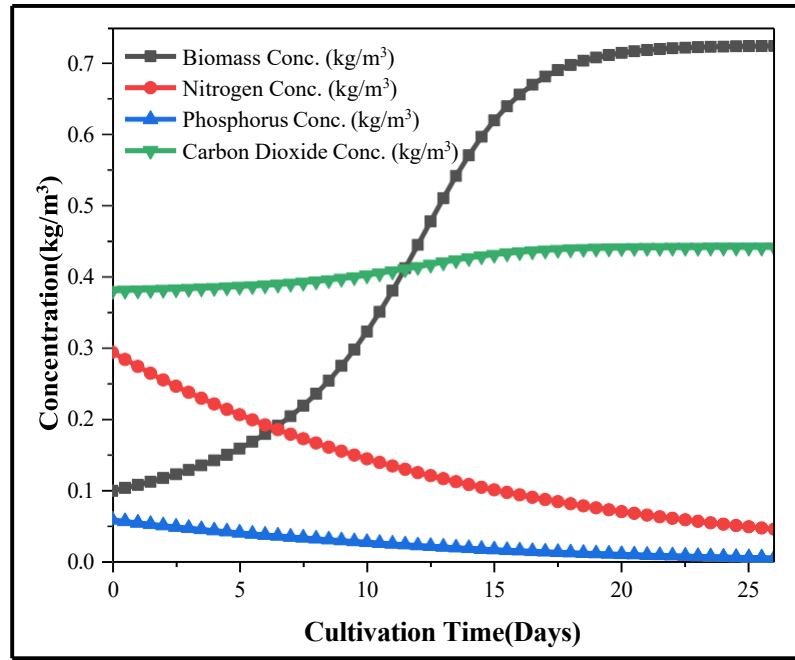


Figure 2.2: Concentration Profile for case 1.

The economic value of the components in **Table 2.3** denotes a significant impact in **Figure 2.2** besides computational aspects on the solution of Eq. 2.12., which can also be processed by more advanced commercial solvers or after some mathematical reformulations. **Table 2.4** summarizes the case study results:

Table 2.4: Results for case 1.

Dilution Coefficient (d^{-1})	Reactor Size	Light Color	Cultivation Medium	Feed Purity	Biomass Concentration (kg/m ³)	Profit (\$)	Profit (\$/kg-dry biomass)
Low ¹	Large	Red	f/2	High	0.7243	4.966	0.7618
Medium	Large	Red	f/2	High	0.6279	3.946	0.6982

¹ Optimum Results for Case 1

High	Large	Red	f/2	High	0.5929	3.576	0.6700
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Although the solution of Eq. 2.12. delivers the first row in **Table 2.4**, additional rows are also calculated to show the impact of the design variables on the profitability, for demonstration purposes to emphasize the solution through simultaneous fashion in an MINLP domain, by fixing dilution coefficient to low and high, as well. Thus, MINLP formulation is further tightened for the corresponding row to a prespecified dilution

coefficient to reduce the degree of freedom in the optimization task.

A case study was conducted to examine the impact of operational parameters, such as the dilution coefficient on production efficiency and economic profitability. The study revealed a significant correlation between dilution coefficient and biomass production, with a 16.23% difference observed between low and medium dilution coefficient.

In order to maximize economic profitability, the preference of low-cost growth media stands out as an important strategy. In this context, f/2 growth medium was determined as the most suitable option due to both its low cost and the high growth performance of the algae species used in this medium. The f/2 medium provides superiority in terms of cost/benefit balance compared to more expensive alternatives such as BG11. Although AM growth medium is advantageous in terms of cost, it has an insufficient effect on the amount of product obtained and therefore on the profitability to be obtained.

In the analysis made in terms of light source, it was determined that the light in the red wavelength has the most suitable spectral properties for the growth of the examined algae species. Red light increases the biomass production efficiency by optimizing the photosynthetic activities of the algae species. In cases where reactor volumes and dilution coefficients are evaluated together, large-volume reactors operating with low dilution coefficients maximize profitability thanks to the high amount of biomass obtained.

In addition to this case study, 7 simulations were conducted including random combinations of design variables and calculating for continuous variables only. A significant drop, compared to **Table 2.4**, is obtained in most cases, as a result of a reduction in degrees of freedom. In addition to this simulation study, the simulation study was repeated many times by assigning random initial values to continuous variables in the process without fixing any process parameters. As a result, the same biomass concentration, profitability and process parameters calculated in **Table 2.5** were calculated. The results of 7 simulations are given as follows:

Table 2.5: Scenarios at different design variables.

Sc. Num.	Light Colour	Dilution Coeff.	Reactor Size	Cultivation Medium	Feed Purity	Profit	Profit/Kg
1	Red	Low	Small	AM	High	4.028	0.611
2	Red	Low	Small	BG11	Low	0.413	0.069
3	Red	High	Large	AM	High	5.2e-9	~0.00
4	Purple	Low	Small	BG11	High	2.1e-10	~0.00
5	Blue	Low	Small	BG11	Medium	0.413	0.069
6	Red	Medium	Small	f/2	Medium	3.854	0.688
7	Red	Low	Medium	f/2	High	3.310	0.762

2.3.2. Case 2: Biomass Concentration Maximization

One typical approach in the synthesis of biochemical reactors is product maximization, a measure of profitability, although indirectly. However, some counter-intuitive implementations would arise once the operational costs or investments bring marginally limited contribution to product synthesis considering their economic value. The second case study aims to maximize the biomass concentration in final time with an objective function, with no economic considerations. Proposed MINLP formulation is given by:

$$\max_{X,P,N,CO_2,C_x,\mu_x,b_i,F_i} X(t_{final}) \quad (2.13a)$$

subject to:

$$\mu_x(t) = \mu^{max} \phi(\alpha \cdot \mu_N(t) + \beta \cdot \mu_P(t) + \delta \cdot \mu_C(t)) \quad (2.13b)$$

$$\mu_N(t) = ([1 - \frac{k_N}{[N(t)]}] \cdot \frac{[X(t)]}{\varphi_N} - \frac{\sum_{i=1}^3 (b_{dil,m} \cdot D_m)}{\mu^{max}} [N(t)]) \quad (2.13c)$$

$$\mu_P(t) = ([1 - \frac{k_P}{[P(t)]}] \cdot \frac{[X(t)]}{\varphi_P} - \frac{\sum_{i=1}^3 (b_{dil,m} \cdot D_m)}{\mu^{max}} [P(t)]) \quad (2.13d)$$

$$\begin{aligned} \mu_C(t) = & k_l \cdot a \cdot [CO_2(t)] (1 - \sum_{i=1}^3 (b_{dil,m} \cdot D_m)) - [C_x(t)] \\ & - [1 - \frac{k_C}{[CO_2(t)]}] \cdot \frac{\mu^{max} [X(t)]}{\varphi_{co2}} \end{aligned} \quad (2.13e)$$

$$\mu^{max} = \sum_{j=1}^3 \sum_{k=1}^3 \sum_{q=1}^3 b_{col,j} \tau_{col,j} b_{feed,k} \omega_{feed,k} b_{med,q} \mu_q^{max} \quad (2.13f)$$

$$\frac{dX}{dt} = \mu_x(t) \cdot [X(t)] - \sum_{m=1}^3 (b_{dil,m} \cdot D_m) \cdot [X(t)] \quad (2.13g)$$

$$\frac{dN}{dt} = -\mu_x(t) \cdot \frac{[X(t)]}{\varphi_N} - \sum_{m=1}^3 (b_{dil,m} \cdot D_m) \cdot [N(t)] \quad (2.13h)$$

$$\frac{dP}{dt} = -\mu_x(t) \cdot \frac{[X(t)]}{\varphi_p} - \sum_{i=1}^3 (b_{dil,m} \cdot D_m) \cdot [P(t)] \quad (2.13i)$$

$$\frac{dCO_2}{dt} = \gamma \frac{dX}{dt} \quad (2.13j)$$

$$\frac{dC_x}{dt} = 0 \quad (2.13k)$$

$$\sum_{i=1}^3 b_{reac,i} = \sum_{j=1}^3 b_{col,j} = \sum_{k=1}^3 b_{feed,k} = \sum_{m=1}^3 b_{dil,m} = \sum_{q=1}^3 b_{med,q} = 1 \quad (2.13l)$$

$$0 \leq X(t), 0 \leq N(t), 0 \leq P(t), 0.2 \leq CO_2(t), 0.25 \leq C_x(t) \quad (2.13m)$$

$$X(0) = 0.1000, N(0) = 0.2944, P(0) = 0.0591, CO_2(0) = 0.3805 \quad (2.13n)$$

The concentration-time graph obtained is presented as follows:

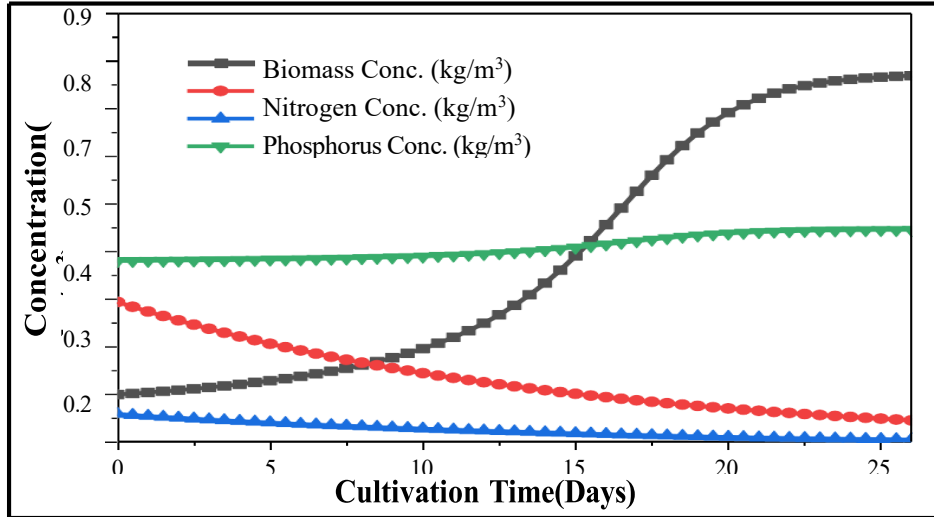


Figure 2.3: Concentration profile of case 2.

In contrast to Case 1, BG11 growth medium was selected, respectively, to maximize the biomass as summarized in **Table 2.6**.

Table 2.6: Result of case 2.

Dilution Coeff. (d^{-1})	Reactor Size	Light Color	Cultivation Medium	Feed Purity	Biomass Concentration	Profit (\$)	Profit (\$/kg- dry biomass)
Low ²	Medium	Red	BG11	Medium	0.7692	0.6277	0.1360
Medium	Medium	Red	BG11	Medium	0.6656	0.3007	0.0753
High	Medium	Red	BG11	Medium	0.6268	0.1783	0.0474

The optimum results for Case 2 is obtained under red light, BG11 and medium purity feed stock are selected. Since the economic concern is not a direct measure in Eq. 2.13a-n , the most expensive medium is introduced although, regardless of its statistical or practical contribution to outcome through impacts on the maximum specific growth rate. Several other simulations were also performed by changing the dilution coefficient to show the impact on biomass and profitability. Similar to **Table2.4** optimization problem is solved under different dilution coefficients, by fixing their corresponding binary variables. Although other design variables are calculated same, by three optimizations a significant biomass decrease is obtained due to reduction in degrees of the problem.

² Optimum Results for Case 2

2.3.3. Case 3: Biomass Concentration Maximization Under Variable Initial Concentration

The models in the first two case studies were developed using initial concentrations estimated from values in the reference study. The third case study also considers the impact of the varying initial concentrations as decision variables for the maximization of the final biomass concentration through:

$$\max_{X,P,N,CO_2,C_x,\mu_x,b_i,F_i} X(t_{final}) \quad (2.14a)$$

subject to:

$$\mu_x(t) = \mu^{max} \phi(\alpha \cdot \mu_N(t) + \beta \cdot \mu_P(t) + \delta \cdot \mu_C(t)) \quad (2.14b)$$

$$\mu_N(t) = ([1 - \frac{k_N}{[N(t)]}] \cdot \frac{[X(t)]}{\varphi_N} - \frac{\sum_{i=1}^3 (b_{dil,m} \cdot D_m)}{\mu^{max}} [N(t)]) \quad (2.14c)$$

$$\mu_p(t) = ([1 - \frac{k_P}{[P(t)]}] \cdot \frac{[X(t)]}{\varphi_P} - \sum_{m=1}^3 (b_{dil,m} \cdot D_m) \mu^{max}) [P(t)] \quad (2.14d)$$

$$\begin{aligned} \mu_c(t) = k_l \cdot a \cdot [CO_2(t)] (1 - \sum_{m=1}^3 (b_{dil,m} \cdot D_m)) - [C_x(t)] \\ - [1 - \frac{k_C}{[CO_2(t)]}] \cdot \frac{\mu^{max}}{\varphi_{CO_2}} \end{aligned} \quad (2.14e)$$

$$\mu^{max} = \sum_{j=1}^3 \sum_{k=1}^3 \sum_{q=1}^3 b_{col,j} \tau_{col,j} b_{feed,k} \omega_{feed,k} b_{med,q} \mu_q^{max} \quad (2.14f)$$

$$\frac{dX}{dt} = \mu_X(t) \cdot [X(t)] - \sum_{m=1}^3 (b_{dil,m} \cdot D_m) \cdot [X(t)] \quad (2.14g)$$

$$\frac{dN}{dt} = -\mu_X(t) \cdot \frac{[X(t)]}{\varphi_N} - \sum_{m=1}^3 (b_{dil,m} \cdot D_m) \cdot [N(t)] \quad (2.14h)$$

$$\frac{dP}{dt} = -\mu_X(t) \cdot \frac{[X(t)]}{\varphi_P} - \sum_{m=1}^3 (b_{dil,m} \cdot D_m) \cdot [P(t)] \quad (2.14i)$$

$$\frac{dCO_2}{dt} = \gamma \frac{dX}{dt} \quad (2.14j)$$

$$\frac{dC_x}{dt} = 0 \quad (2.14k)$$

$$\sum_{i=1}^3 b_{reac,i} = \sum_{j=1}^3 b_{col,j} = \sum_{k=1}^3 b_{feed,k} = \sum_{m=1}^3 b_{dil,m} = \sum_{q=1}^3 b_{med,q} = 1 \quad (2.14l)$$

$$0 \leq X(t), 0 \leq N(t), 0 \leq P(t), 0.2 \leq CO_2(t), 0.25 \leq C_x(t) \quad (2.14m)$$

$$X(0) \leq 0.25, N(0) \leq 0.35, P(0) \leq 0.1, CO_2(0) \leq 0.48 \quad (2.14n)$$

where initial conditions are tightened by an inequality constraint, unlike Eq. 2.12 and Eq. 2.13. The optimization result concentration profile is shown in **Figure 2.4**. **Figure 2.4** shows that the initial concentrations of biomass, nitrogen, phosphorus, and carbon dioxide were calculated as 0.1999 kg/m³, 0.2771 kg/m³, 0.0990 kg/m³, and 0.4654 kg/m³, respectively. The medium reactor size with a low dilution coefficient was calculated as the optimum experimental conditions with BG11 growth medium, the lowest purity feed stream, and red light. At the final time, the biomass concentration reached 0.9804 kg/m³, the highest among all cases

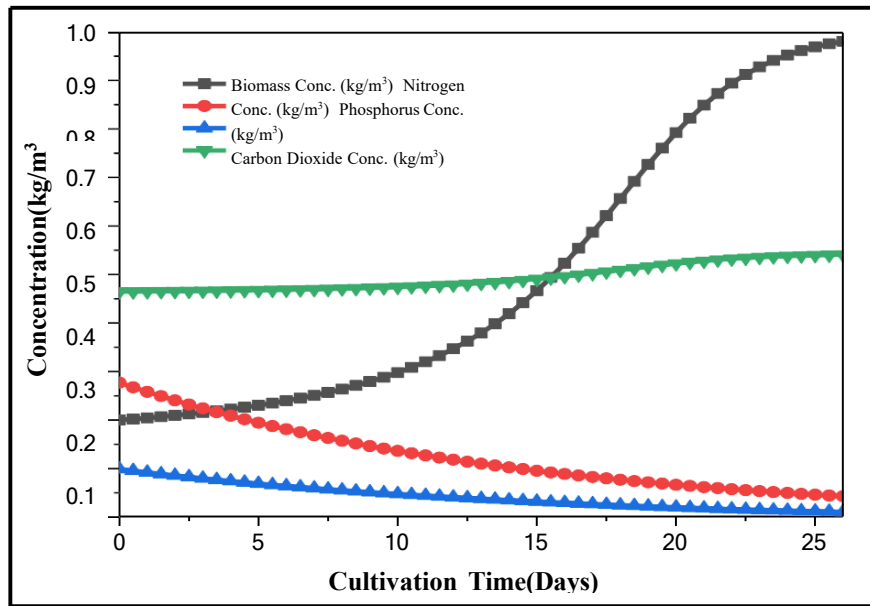


Figure 2.4: Concentration profile of case 3.

2.3.4. Comparison of Case Studies

Table 2.7 includes the results of discrete decisions on three cases and provides insight on how they might differ based on the process requirements in such a complex process of microorganisms:

Table 2.7: Summary of case studies.

Case ID	Feed Impurity	Reactor	Dilution Coefficient	Light Color	Cultivation Medium	Biomass Concentration	Profit	Profit/kg Dry Biomass
1	High	Large	Low	Red	f/2	0.7243	4.9660	0.7618
2	Medium	Medium	Low	Red	BG11	0.7692	0.6277	0.1360
3	Low	Medium	Low	Red	BG11	0.9804	1.2943	0.2203

Case 1 aims to maximize profit and a cost-effective medium, f/2, is a better choice based for profitability under highest purity feed in the largest available reactor under low dilution. BG11 medium, which is known to support high cell densities, is preferred in Case 2 and Case 3 to maximize the biomass regardless of economic considerations. When comparing case studies 1 and 2, the profitability decreases from 0.7618 \$/kg dry biomass to 0.1360 \$/kg biomass, demonstrating the importance of wise decision in the

process design and synthesis. This decrease can be explained as the effect of the chosen cultivation medium cost on profitability. In Case 3, the initial concentrations are also decision variables, introducing more flexibility to optimization problem. The results of this case would likely show how varying the initial concentration of the microalgae affects growth and productivity, with higher initial concentrations leading to higher cell densities and lower growth rates. The initial concentration was increased two and times, approximately, resulting in an increase in biomass concentration of 27.46% at the final time, compared to Case 2. **Figure 2.5** provides a comparison of biomass concentrations for three cases.

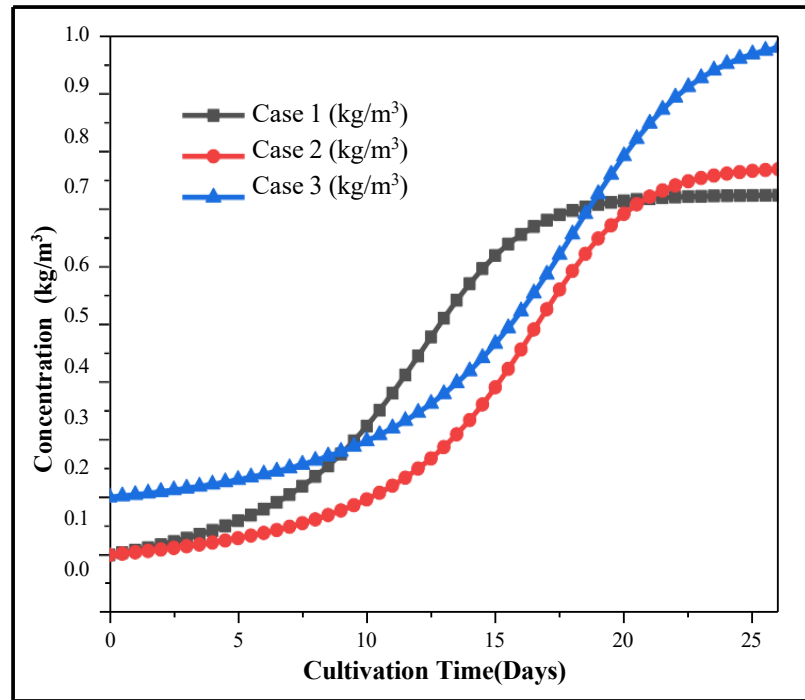


Figure 2.5: Biomass concentration profile for all cases.

2.4. Conclusion

Biochemical processes, including algae growth and processing, are often non-linear with complex and coupled interactions, which require significant modeling effort calling for a comprehensive experimental setup and subsequent computational tasks. Furthermore, these processes might experience high sensitivity to environmental conditions, unmeasured disturbances and unknown driving forces, delivering undesired or poor-performance outcomes. Thus, modeling tasks should incorporate practical issues with data availability for the subsequent purposes including the

optimization and process operability. Those purposes mostly are dynamic and need to be updated based on new regulations or market conditions both in terms of feedstock prices and other operational costs with a wide spectrum. In turn, a mixed integer formulation to address the transient patterns in the biochemical process becomes an important research area to handle both the continuous operational variables and selection of design variables with discrete nature, due to market availability or variable nature.

The MINLP formulation in this study employs a complex and nonlinear algae growth model whose parameters are identified from experimental data. The parameter identification task is performed through a constrained nonlinear optimization task, which might suffer from local optimality issues and would be improved once additional data are collected at different operating conditions with spatial or temporal variation. Statistical identifiability would also be favored by including other process variables in the measurement variables to avoid multiplicity issues for a better approximation of the model and plant compatibility, besides reformulation tasks related to nonconvex terms.

While simultaneous MINLP formulation, addressing the continuous and the discrete variables, brings about significant potential to exploit the capability of the process. Furthermore, current results are obtained through open-source BONMIN solver without proper treatment of the original problem, which carry significant nonlinearity and nonconvexity. However, tightened constraints enabled convergence to same optimums after several randomly generated initial guesses unless they are outside the feasible region, in current simulation bounds and our cases. On the other hand, global optimality is still not ensured, as design variables have significant impact on the process performance and superior methods which decompose the original problem into subsequent but coordinated problems through sophisticated reformulations and approximations might be required. However, proposed formulation, despite locality, delivers satisfactory results and is useful to demonstrate the contribution of the general framework and the approach. Thus, more realistic modeling, development of an experimental setup for the data collection or advanced mathematical tasks to favor global optimality are considered out of the scope of the study.

Proposed formulations are solved through Python/PYOMO, which has the integration capability to many open source and commercial solvers. In addition, built-in

subroutines enable automatized discretization for the simultaneous solutions to be handled by the solvers for subsequent reformulations or evaluations. Current discretization architecture provided satisfactory accuracy once the set of DAEs are solved through common solvers in MATLAB. Thus, numerical accuracy is ensured in the model solution, for reliability in optimization tasks. With computationally friendly formulation in this study, the results are obtained within a small time and would still bring insight at scale-up considerations or industrial process design at different scales.

The case studies show the potential tradeoff between the profitability and production rate once the process costs are considered. In practice, there are many manipulated variables and design variables with a potential to favor biomass growth; however, their contribution would be uncompensated depending on the relative prices. The results in this study are obtained by a specific set of prices and would change once they change. Moreover, those prices are for demonstration purposes and do not include a detailed analysis on compatibility to actual market conditions. In practice, those prices have a strong dependency on the region where the algae is processed and seasonal issues in to consider demands and supply from competitors.

In the problem formulation, the discrete and continuous nature of a variable might be evaluated based on practical issues, rather than theoretical considerations. For instance, the feed impurity in this study is a selection, and thus discrete, variable with three options to be used in the optimization. This might be the case in engineering implementations once the feedstock is obtained from a set of different vendors providing a fixed composition. In turn, once the blending of those feedstocks is not available, the variable representation through binary variable is a better and more representative approach, although a significant computational complexity is introduced in contrast to the case where it is defined by a continuous variable. Similarly, reactor selection task is represented by binary variables to represent the availability of particular reactor sizes at the market where specific sized production is not applicable. A comparison or contribution of representation of these variables through continuous nature is out of the scope of this study; but could be accomplished easily once needed.

3. A MIXED-INTEGER DYNAMIC AND STOCHASTIC ALGAE PROCESS OPTIMIZATION

3.1. 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 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 [49].

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 Linear 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 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 [50], [51].

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 [52].

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 [34], [52].

In contrast to deterministic approach, models that deal with uncertainty are crucial in performing optimization under uncertain conditions [53]. 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, reactors and catalyst efficacy. Thus, it is crucial to employ stochastic modelling in the analysis of process systems [54].

In this study, the dynamic optimization of *Nannochloropsis Oculata* algae growth, calculating optimal process conditions and maximizing biomass profit under economic uncertainty was analyzed, and the effect of dynamic and non-linear constraints on the process were also investigated. For realistic modelling and optimization 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 optimization, risk analysis and decision-making strategies.

3.2. Methodology

This study aims to develop a stochastic MINLP model for *Nannochloropsis Oculata* algae by updating Tijani et al.'s previous model [40]. The mathematical model which aims to maximize the average profit is given by:

$$\min_{X,P,N,CO_2,C_x,\mu_x,b_i,r_i,h_i,F_i} \frac{\sum_{s=1}^{s_T} (E[s] - R[s])}{s_T} \quad (3.1a)$$

3

$$R[s] = X(t_f) \cdot (\sum_{i=1}^3 b_i V_{r,i}) \cdot (p_f[s] \cdot f_f[s] + p_{fr}[s] \cdot f_{fr}[s]) \quad (3.1b)$$

$$E[s] = X(t_f) \cdot ((\sum_{i=1}^3 b_i V_{r,i}) \cdot (\sum p_{oc}[s]) + (p_w[s] \cdot \sum_{i=1}^3 b_i V_{r,i})) \quad (3.1c)$$

subject to:

$$\mu_x(t) = \mu^{max} \cdot \phi \cdot (\alpha \cdot \mu_N(t) + \beta \cdot \mu_P(t) + \delta \cdot \mu_c(t)) \quad (3.1d)$$

$$\mu_N(t) = ([1 - \frac{k_N}{[N(t)]}] \cdot \frac{[X(t)]}{\varphi_N} - \frac{\sum_{i=1}^3 (b_i D_i)}{\mu^{max}} [N(t)]) \quad (3.1e)$$

$$\mu_P(t) = ([1 - \frac{k_P}{[P(t)]}] \cdot \frac{[X(t)]}{\varphi_P} - \frac{\sum_{i=1}^3 (b_i D_i)}{\mu^{max}} [P(t)]) \quad (3.1f)$$

$$\mu_c(t) = k_l \cdot a \cdot \frac{[CO_2(t)](1 - \frac{\sum_{i=1}^3 (b_i D_i)}{\mu^{max}}) - [C_x(t)]}{[X(t)]} - [1 - \frac{k_c}{[CO_2(t)]}] \cdot \frac{[X(t)]}{\varphi_{co2}} \quad (3.1g)$$

$$\frac{dX}{dt} = \mu_x(t) \cdot [X(t)] - \sum_{i=1}^3 (b_i D_i) \cdot [X(t)] \quad (3.1h)$$

$$\frac{dC_x}{dt} = 0 \quad (3.1i)$$

$$\frac{dP}{dt} = -\mu_x(t) \cdot \frac{[X(t)]}{\varphi_P} - \sum_{i=1}^3 (b_i D_i) \cdot [P(t)] \frac{dCO_2}{dt} = \gamma \frac{dX}{dt} \quad (3.1j)$$

$$\frac{dCO_2}{dt} = \gamma \frac{dX}{dt} \quad (3.1k)$$

$$\frac{dN}{dt} = -\mu_x(t) \cdot \frac{[X(t)]}{\varphi_N} - \sum_{i=1}^3 (b_i D_i) \cdot [N(t)] \quad (3.1l)$$

$$\sum_{i=1}^3 b_i = 1 \quad (3.1m)$$

$$V_i = \pi r_i^2 h_i, D_i = \frac{F_i}{V_i}, r_{i,min} \leq r_i \leq r_{i,max}, h_{i,min} \leq h_i \leq h_{i,max} \quad (3.1n)$$

$$\mu^{max} \geq \mu_x(t) \quad (3.1o)$$

$$X(0) = 0.100, N(0) = 0.290, P(0) = 0.049, CO_2(0) = 0.31 \quad (3.1p)$$

$$0.2 \leq CO_2(t), 0.25 \leq C_x(t) \quad (3.1r)$$

$$\frac{r_i}{h_i} \geq 0.2, \frac{r_i}{h_i} \leq 0.9 \quad (3.1s)$$

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}); $k_l \cdot a$ coefficient was limited to the range of (107-156) d^{-1} based on the experimental data by Tijani et al. [40].

α , β and δ are weighting factors and determined as 0.197 0.079 and 0.441 respectively.

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; b_i is 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 ”.

The model is solved by using Basic Open-source Nonlinear Mixed-Integer programming (BONMIN) solver which is capable for Mixed Integer Quadratically

Constrained Program (MIQCP) and MINLP. Parameter values which are used in mathematical models are given in the following table:

Table 3.1: Growth parameter values.

Parameter	Value	Unit	Parameter	Value	Unit
μ^{max}	0.3110	d ⁻¹	D_2	0.0800	d ⁻¹
k_N	0.0417	kgN/m ³	D_3	0.0900	d ⁻¹
φ_N	851.81	kgX/kgN	D_4	0.1100	d ⁻¹
k_P	0.0006	kgP/m ³	D_5	0.1200	d ⁻¹
φ_P	192.92	kgX/kgP	α	0.1970	--
k_C	0.2862	kgCO ₂ /m ³	β	0.0790	--
φ_{co2}	0.0082	kgX/kgCO ₂	δ	0.4410	--
$k_l \cdot a$	127.64	d ⁻¹	ϕ	0.8570	--
D_1	0.1000	d ⁻¹	γ	0.0890	--

3.3. Results

Algae growth profile under consideration includes a 12-day exponential growth period ended due to extinction of substrate. **Figure 3.1** is obtained through a deterministic approach where the economic considerations are fixed (Kivanc et al.,2023).

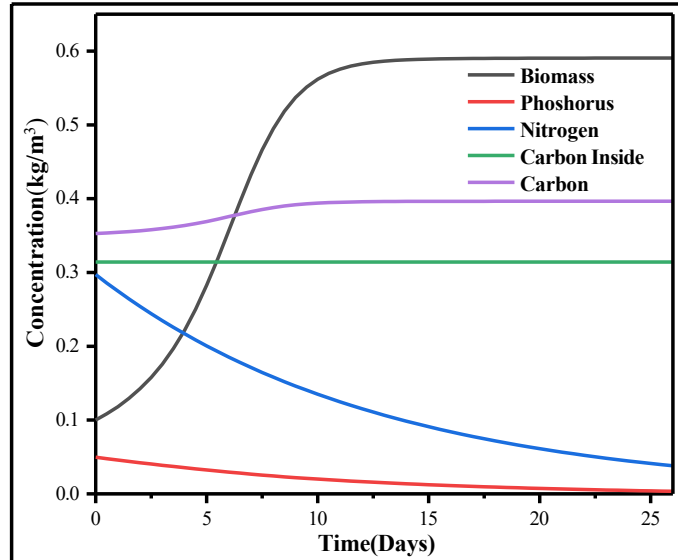


Figure 3.1: Concentration profiles of nutrients and biomass.

Table 3.2 displays 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 data gathered, 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 3.2: Result of simulations.

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

Also calculated dimensions are given as follows:

Table 3.3: Continuation of results.

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%. 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.

Figure 3.2 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.

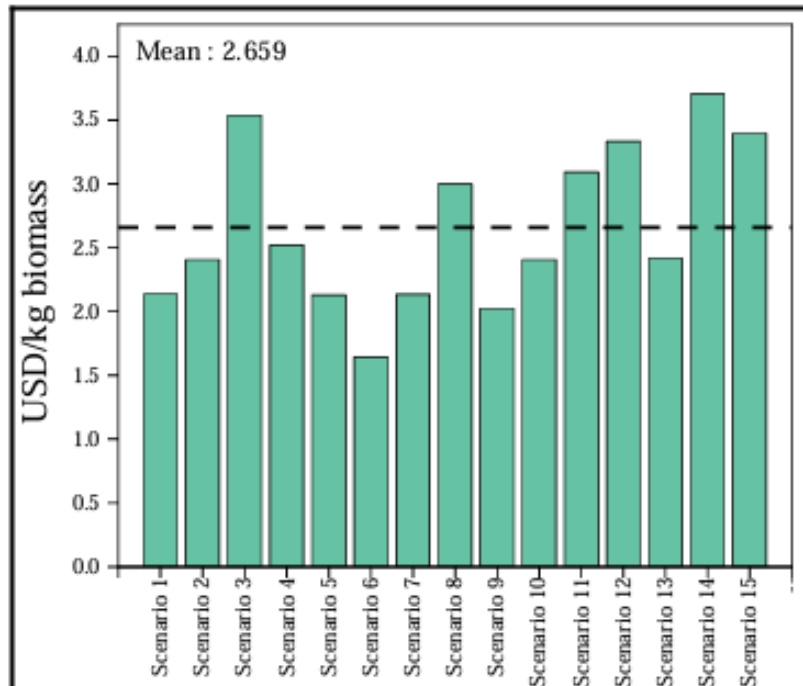


Figure 3.2: Profits of scenarios

Upon evaluation of the results, the average profit was found to be 2.659 USD/kg of biomass. The highest profit was obtained in the 14th scenario, with 3.704 USD/kg of biomass, while the lowest profit was observed in the 6th scenario, with 1.643 USD/kg of biomass. These results demonstrate the impact of various economic scenarios on business profitability.

The 14th scenario yielded the highest profit, indicating positive conditions for the business and increased profitability. Conversely, the 6th scenario resulted in the lowest profit, 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.

3.4. Conclusion

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.

4.DYNAMIC AND STOCHASTIC OPTIMIZATION of ALGAE CULTIVATION PROCESS

4.1. Introduction

Energy plays a crucial role in the sustainability of our lives and is essential for nations to achieve political and economic independence [55], [56]. As it is expected that energy consumption increase from 550 EJ to 865 EJ by 2040, the depletion of limited resources like fossil fuels is rapidly increasing [57]. Furthermore, the accumulation of harmful gases such as CO₂, NO_x, and SO_x in the atmosphere is a cause of global climate problems [58], [59]. Scientists are conducting studies on sustainable energy production, focusing on renewable energy sources like hydrothermal, geothermal, solar, and biomass [60]. Energy sources from biomass can be classified into the first, second, and third-generation sources [61]. First-generation energy sources are obtained from food products like sugar, starch, and maize, which pose ethical and sustainability issues [62]. Second-generation energy sources, such as inedible plant wastes, are suitable for producing biofuels and are cheap to produce [63]. Third-generation energy sources, including organisms like microalgae, macroalgae, and cyanobacteria, offer advantages such as short production times, limited space requirements, biofuel production, and photosynthesis [60].

Algae use sunlight and CO₂ to transform the inorganic materials into organic nutrients [64], [65]. Further processing enables the production of organic nutrients such as biofuel, biohydrogen, and bioethanol with their products, making algae promising third-generation energy sources for agriculture, food, energy, and other sectors [58], [66]. Algae are promising sources for biofuel production because they have adaptable growth conditions, rapid growth, photosynthetic efficiency, high lipid content, CO₂ fixation, and wastewater utilization [67]–[70]. On the other hand, there are also some disadvantages such as low productivity, challenges in large-scale production, high production costs, and challenges in product purification [67], [71]. Furthermore, algae present various opportunities, including technological advancements, commercialization, a share in the energy market, CO₂ capture, and biodiesel production [71]. Intensive research and development studies on algae are being conducted by scientists, government energy agencies, and energy companies in line

with these benefits and opportunities to move towards large-scale production.

The algae cultivation process is at the heart of the algae-driven energy economy and can be divided into two main categories, open and closed systems. Open systems include open basins, raceways, and tanks. Closed systems are systems that are classified as vertical and horizontal according to their orientation, and as flat plate or helical according to their geometry [63]. Light transmission is usually obtained through the transparent materials in the design of closed systems [72]. There are advantages and disadvantages to both concepts when comparing open and closed systems. Construction and operating costs are generally lower for open systems. In this respect, they have lower energy consumption and costs and are more suitable for the production of food supplements such as protein and carotene [57]. However, open systems also have several disadvantages, including contamination risk, the need for land for investment, evaporation of water from the culturing medium, issues with light penetration, uncertainties due to weather conditions, and challenges in process control [57]. Closed systems are more commonly used in industrial applications and some of their advantages are reduced water evaporation and CO₂ loss, obtaining products with less uncertainty under stable operating conditions, more robust and simpler process control, high productivity, and efficiency. On the negative side, high investment costs, biofilm formation resulting in decreased light penetration, and problems with scaling up are typical issues [57]. Batch systems, semi-batch systems, and continuous systems are all in use. For reasons such as ease of installation, small-scale operation, and low risk of contamination, batch systems are the most preferred reactor types for biofuel production [57].

For close systems, a wise design and operation for any algae cultivation process is necessary to increase efficiency, biomass yield, economic viability, and environmental sustainability. In this perspective, several studies have considered mathematical modeling and optimization to systematically study the best processing conditions for both open and closed systems. For closed systems, Al Ketife et al. developed a comprehensive mathematical model for *Chlorella Vulgaris* to determine the optimum nutrient concentration and light intensity in a glass cylindrical photobioreactor [73]. A model, calibrated based on experimental data of feed gas CO₂ concentration, initial nutrient concentration, and irradiation intensity, has been developed for the simulation of dynamic behavior in terms of biomass growth, nutrient absorption, and removal from a water stream. As a function of biomass concentration, the calibrated model

successfully predicted algal growth, nutrient removal, and average light intensity within the biomass mass. Furthermore, Zhou et al. investigated the effect of a limited concentration of nutrients or light on the growth rate and determined the optimum value of the dilution ratio and the concentration of inorganic nitrogen [74]. See et al. calculated the kinetic parameters of *Botryococcus Braunii* algae based on the Monod model [75]. Haghpahan et al. used mixed-integer nonlinear programming to optimally select the processing equipment that minimized the total annual cost as well as environmental impacts within a multi-objective superstructure optimization framework [76]. Moreover, Rizwan et al. proposed a two-stage deterministic model for the design of a microalgae-based biofuel and co-product supply chain network. In their study, the first stage selected the best location for plant installation, while the second stage maximized profit while minimizing environmental impact [77]. Unlike traditional optimization methods, del Rio-Chanona et al. developed a hybrid stochastic algorithm by using deep learning and testing complex hydrodynamic and biochemical kinetic models [78]. Kumar et al. used images and measurement data collected from the reactor at certain time intervals to perform image processing [79]. Doan et al. proposed a new time-dependent reinforcement learning method with state prediction by long short-term memory networks to optimize the dry weight yield of *Spirulina* sp. [80]. Sultana et al. presented Bayesian optimization algorithm-based machine learning techniques such as artificial neural networks and support vector regression as a potential tool for modeling biodiesel production from algae [81]. Final study is conducted by [82], a simulation model was developed to evaluate the impact of decision variables on production yield in horizontal and vertically stacked horizontal tubular reactors. The model utilized inputs such as reactor dimensions, dynamic sunlight patterns, and algae growth characteristics.

In open systems, Chuka-ogwude et al. investigated the effect of turbidity on *Chlorella* sp. algae growth and optimized the depth of the cultivation pond for higher productivity under constraints [83]. Babazadeh et al. investigated the application of a data environment analysis approach in the selection of the best sites for microalgae cultivation through ecological and economic factors [84]. Kazemi et al. used data envelopment analysis, energy economic analysis, and life cycle assessment (LCA) to optimize the energy and environmental impacts of microalgae cultivation [85]. Furthermore, [86] present an integrated LCA framework for synthesizing microalgae

cultivation systems using a multi-objective linear program formulation. In the model, individual objective functions were summed and weighted using the analytic hierarchy process. Sajid et al. conduct an economic analysis of a biodiesel plant that produces 45000 tons of biodiesel per year from *Jatropha* oil using a homogeneous base-catalyzed process [87]. To address uncertainties in cost and revenue estimates, the study develops a risk analysis methodology and applies it to a biodiesel example. Probabilistic cost-benefit analysis is performed to address economic risks, providing a precise indication of the return period over the investment period.

Although these studies have addressed many important aspects of algae production and optimization from both economic and environmental perspectives deterministically, the uncertainty surrounding measurement errors, environmental variability, or in-system fluctuations is overlooked. Other existing studies that considered uncertainties in algae production mainly focused on the uncertainties involving surrogate model predictions and demand and/or delivery time uncertainties in microalgae-based supply chains [25], [88]–[90]. Even though scenario-based stochastic programming is a well-established method to model and study decision-making uncertainty with a risk-neutral approach, it has not been fully explored for algae production to the best of the authors' knowledge [54], [91]–[93]. Motivated by this, we formulate a two-dimensional dynamic algae batch bioreactor and quantify the uncertain effects of light intensity, as well as nitrogen and phosphorous concentrations in the culturing medium on the lipid productivity of the *Chlamydomonas Reinhardtii*. We use the Python/Pyomo framework to discretize and solve the resulting process of partial differential algebraic equations (PDAEs) and use scenario analysis to characterize uncertain effects [44], [94], [95]. We create 30 different scenarios involving inhibition and saturation constants assuming normal probability distribution and maximizing the expected lipid productivity across all scenarios under case-dependent selectivity constraints. Our study offers a distinct and more comprehensive analysis for understanding the uncertain effects of key parameters on lipid productivity and algae growth by integrating stochastic programming and spatiotemporal modeling of the bioreactor.

4.2. Methodology

4.2.1. Spatiotemporal Model for the Algae Bioreactor

Various mathematical expressions have been developed to express nutrient-cell interactions and understand reaction networks [96]. These can be examined under two main headings, primary and secondary models [97]. Primary models, such as Malthusian, Gompertz, and Logistic models, examine algae growth rate and reaction kinetics using fewer parameters. These models are simplified with fewer parameter usage but have a higher prediction error compared to secondary models. Primary models are essential for understanding the interactions between nutrients and cells in algae cultivation [97].

Secondary models consider the interaction of growth rate with environmental factors. They can be classified as single or multiple effects, with single effects expressing the effect of one environmental factor on growth rate, and multiple expressions expressing the simultaneous effects of multiple factors [97]. These models can be categorized under three main headings: Monod, Haldane-Andrews, and Droop models [41]. Other models include Martinez-Sancho, Geider, and Molina-Grima [96]. The Monod, Haldane-Andrews, and Droop models are categorized based on their advantages, disadvantages, study purpose, and model suitability for the chosen algae variety [96].

The Monod model is commonly used for describing growth rate expressions based on a single environmental factor and low and adjustable nutrient concentrations [41]. However, it is insufficient for high-nutrient concentration reactors, where microalgae can continue growth despite resource depletion [41], [96]. As a result, different mathematical models have been developed. One of these developed models is the Haldane-Andrews model, developed to explain organism growth at high nutrient media concentrations, which is crucial for determining initial conditions for maximizing cell density and productivity [96], [98]. The Droop model, on the other hand, expresses the intrinsic concentration of nutrient quantity relative to carbon-based biomass [32]. However, the Droop model has a challenge with its mathematical formulation, as it can reach an unrealistic value when the growth rate is equal to the maximum [41]. The models are expressed mathematically as follows [32], [41], [96]:

Table 4.1: Reaction kinetic models.

Model Type	Expression	
Monod	$\mu_m = \mu_{max} \frac{[A]}{K_A + [A]}$	(4.1)
Andrews-Haldane	$\mu_H = \mu_{max} \frac{[A]}{[A] + K_A + \frac{[A]^2}{K_{iA}}}$	(4.2)
Droop	$\mu_D = \mu_{max} \left(1 - \frac{Q_0}{q}\right)$	(4.3)

In the equations, μ_m , μ_H and μ_D are the growth rate (time⁻¹) for the Monod, Haldane-Andrews, and Droop model, respectively; μ_{max} is the maximum growth rate (time⁻¹); $[A]$ is the concentration (g/L) of any component (e.g., nitrogen, phosphorus); K_A is the saturation constant (g/L); K_{iA} is the inhibition constant (g/L); Q_0 is the minimum cell quota; q is the cell quota.

Researchers have studied the combined effects of these components, in addition to individual contributions, by using nutrient media from environments such as wastewater, salt water, or chemical solutions [99]. These studies, which are referred to as multi-substrate models, delivered more realistic predictions [41]. Multi-substrate models can be classified into interactive, additive, and non-interactive models [96]. This study used an interactive system that simulated growth using the Andrews-Haldane kinetic growth model, which considers that the overall growth rate is influenced simultaneously by two or more growth parameters. Interactive models show multi-effects of environmental factors on the overall growth rate and are generally expressed as [98]:

$$\mu = \mu_{max} \cdot [f(A_1) \cdot f(A_2) \dots f(A_n)] \quad (4.4)$$

where $f(A_n)$ is the function to include the effect of environmental factors on the growth rate; n refers to environmental factors. In addition to the concentrations of the compounds in the nutrient medium, equations expressing the time-dependent changes of ambient conditions such as light, temperature, and pH and their effects on growth rate have also been developed. The behavior of the light intensity depending on the location is usually expressed with the Beer-Lambert equation and given by [100]:

$$I(l) = I_0 \cdot e^{-\sigma \cdot X \cdot l} \quad (4.5)$$

In Equation 4.5, $I(l)$ is light intensity ($\mu\text{mole}/\text{m}^2 \cdot \text{s}$) depending on location; I_0 is the light intensity ($\mu\text{mole}/\text{m}^2 \cdot \text{s}$) on the reactor surface; σ extinction coefficient ($\text{L}/\text{m} \cdot \text{g}$); X is the biomass concentration (g/L); l represents the reactor position (m). In the literature, there are equations derived from the Beer-Lambert equation describing the behavior of light in different ways. The opaque Beer-Lambert culture medium equation and hyperbolic light expression can be given as examples of these equations as shown in **Table 4.2**.

Table 4.2: Light intensity distribution expressions [100].

Model Type	Expression	
Modified Beer-Lambert in Non-transparent Medium	$I(l) = I_0 \cdot e^{[-(k_w \cdot k_x \cdot X) \cdot l]}$	(4.6)
Hyperbolic	$I(l) = \frac{I_0}{(K_L \cdot l + 1)^{n_1} \cdot (K_X \cdot X \cdot l + 1)^{n_2}}$	(4.7)

The k_w , k_x , K_L , K_X , n_1 , and n_2 in Equation 4.6 and 4.7 represent experimental parameters [101], [102].

The isothermal spatiotemporal photobioreactor model is composed of equations in Eq. 4.8-4.20. Proposed formulation implements pseudo-steady state assumption on light due to significant differences in time constant scales related to material and light dynamics, enabling the solutions through coupled ODEs with different independent variables although the time and spatial coordinate is related through algebraic growth rate expressions as shown in:

$$\frac{\partial X(t, x)}{\partial t} = \mu_x(t, x) \cdot X(t, x) \quad (4.8)$$

$$\frac{\partial L(t, x)}{\partial t} = \mu_L(t, x) \cdot X(t, x) \quad (4.9)$$

$$\frac{\partial S(t, x)}{\partial t} = -\frac{1}{Y_S^X} \mu_x(t, x) \cdot X(t, x) - \frac{1}{Y_S^L} \mu_L(t, x) \cdot X(t, x) \quad (4.10)$$

$$\frac{\partial N(t, x)}{\partial t} = -\frac{1}{Y_N^X} \cdot \mu_x(t, x) \cdot X(t, x) \quad (4.11)$$

$$\frac{\partial I(t, x)}{\partial x} = k_1 \cdot I(t, x) + k_2 \cdot X(t, x) \quad (4.12)$$

where t is the time; x is the spatial coordinate in the reactor; $\mu_x(t, x)$ is the biomass growth rate (h^{-1}) at process time t and reactor location x ; $X(t, x)$ is the biomass concentration (gX/L) at t and x ; $L(t, x)$ is the lipid concentration (g/L) at t and x ; $\mu_L(t, x)$ is the lipid accumulation (growth) rate (h^{-1}) at t and x ; $S(t, x)$ is the substrate concentration (gS/L) at t and x ; Y_S^X is the yield coefficient for oil-free biomass production with respect to the substrate (gX/gS); Y_S^L is the yield coefficient for lipid production with respect to the substrate (gL/gS); $N(t, x)$ is the nitrogen concentration (gN/L) at t and x ; Y_N^X is the yield coefficient for oil-free biomass production with respect to the nitrogen (gX/gN); $I(t, x)$ is the light intensity ($\mu\text{mole/m}^2.\text{s}$) at t and x ; and $k_1(\text{m}^{-1})$ and $k_2(\text{L}.\mu\text{mole/g.m}^3.\text{s})$ are constants for light intensity [23]. The yield coefficients and the light intensity constants are given in **Table 4.3**.

Equations 4.8 and 4.9 express the biomass and lipid accumulations, whereas Equations 4.10 and 4.11 express the substrate and nitrogen consumption along the reactor with time. The change in the light intensity across the reactor is also linearly represented in Equation 4.12 which is composed of the effect of light absorption inherent in water or any liquid (first term) and the self-shading effect that develops due to biofilm formation and increasing biomass concentration due to algae growth (second term). Here, we opted for a linear expression of Equation 4.12 to avoid creating an intractable equation solution task. We also assume that the pH in the photobioreactor is well-maintained and constant. In addition to the aforementioned equations, we express the effect of environmental factors on the growth expression using the following equations [23]:

$$\mu_x(t, x) = \mu_{X, \max} \cdot f_x(S) \cdot f_x(N) \cdot f_x(I) \quad (4.13)$$

$$\mu_L(t, x) = q_{L, \max} \cdot f_L(S) \cdot f_L(N) \cdot f_L(I) \quad (4.14)$$

$$f_x(S) = \frac{S(t, x)}{S(t, x) + K_{XS} + \frac{S(t, x)^2}{K_{iXS}}} \quad (4.15)$$

$$f_x(N) = \frac{N(t, x)}{N(t, x) + K_{XN} + \frac{N(t, x)^2}{K_{iXN}}} \quad (4.16)$$

$$f_x(I) = \frac{I(t, x)}{I(t, x) + K_I + \frac{I(t, x)^2}{K_{iI}}} \quad (4.17)$$

$$f_L(S) = \frac{S(t, x)}{S(t, x) + K_{LS} + \frac{S(t, x)^2}{K_{iLS}}} \quad (4.18)$$

$$f_L(N) = \frac{K_{iNL}}{N(t, x) + K_{iNL}} \quad (4.19)$$

$$f_L(I) = \frac{I(t, x)}{I(t, x) + K_I + \frac{I(t, x)^2}{K_{iI}}} \quad (4.20)$$

where $\mu_{X,max}$ is the maximum growth rate (h^{-1}); $f_x(S)$ is the function expressing the effect of substrate concentration on the biomass growth rate; $f_x(N)$ is the function expressing the effect of nitrogen concentration on the biomass growth rate; $f_x(I)$ is the function expressing the effect of light intensity on the biomass growth rate; K_{XS} is the substrate saturation constant for biomass (gS/L); K_{iXS} is the substrate inhibition coefficient for biomass (gS/L); K_{XN} is the nitrogen saturation coefficient for biomass (gN/L); K_{iXN} is the nitrogen inhibition coefficient for biomass (gN/L); $q_{L,max}$ is the maximum lipid growth rate (h^{-1}); $f_L(S)$ is the function expressing the effect of substrate concentration on the lipid growth rate; $f_L(N)$ is the function expressing the effect of nitrogen concentration on the lipid growth rate; $f_L(I)$ is the function expressing the effect of light intensity on the lipid growth rate; K_{LS} is the substrate saturation constant for lipid (gS/L); K_{iLS} substrate inhibition coefficient for lipid (gS/L); K_{iNL} is the nitrogen inhibition coefficient for lipid (gN/L); K_I is the saturation coefficient for lipid and biomass accumulation ($\mu\text{mole/m}^2\text{s}$); K_{iI} is the coefficient of inhibition for lipid and biomass deposition ($\mu\text{mole/m}^2.\text{s}$). The values of the coefficients are provided in **Table 4.3**. Next, we discuss our dynamic optimization strategy to find the optimal operating conditions for the algae bioreactor in detail.

Table 4.3: Parameter values defining the photobioreactor model [23].

Parameter	Value	Units	Parameter	Value	Units
Y_S^X	1.3500	gX/gS	K_{XN}	0.0812	gN/L
Y_S^L	0.0480	gL/gS	K_{iXN}	0.6250	gN/L
Y_N^X	5.1623	gX/gN	$q_{L,max}$	0.1512	h ⁻¹
k_1	0.1996	m ⁻¹	K_{LS}	4.9155	gS/L
k_2	9.4830	L.μmole/g.m ³ .s	K_{iLS}	0.1375	gS/L
$\mu_{X,max}$	0.2750	h ⁻¹	K_{iNL}	380.3100	gN/L
K_{XS}	0.0624	gS/L	K_I	45.5000	μmole/m ² .s
K_{iXS}	12.4000	gS/L	K_{il}	297.7500	μmole/m ² .s

4.2.2. Dynamic Formulation and Deterministic Optimization

Our goal is to identify the optimal growth medium in the photobioreactor that maximizes the algae lipid productivity at the final time and center of the reactor, which is mathematically expressed as follows:

$$\max_{S,N,L,X,I} \frac{L(t_f, x_0) - L(t_0, x_0)}{t_f - t_0} \quad (4.21)$$

where t_f is the final process time (hour); t_0 is the initial process time (hour); and x_0 represents the reactor target position (meter). Although we chose the reactor center as the target region for optimization, our two-dimensional model allows flexibility to optimize for any reactor depth. The center of the reactor is an ideal location to observe the average light penetration effects since the bottom will suffer from very low light penetration and the algae closer to the edges of the reactor will benefit from high light exposure.

This objective function is further subject to the dynamic model expressions provided in Equations 4.8-4.20 as well as additional constraints defining the boundary conditions limiting these growth rate expressions, boundary conditions used in estimating initial conditions, as well as constraints on the concentrations of substrate, nitrogen, and lipid at final time. The resulting dynamic program is expressed as:

$$\begin{aligned} & \max_{S,N,L,X,I} \frac{L(t_f, x_0) - L(t_0, x_0)}{t_f - t_0} \\ & \text{subject to:} \end{aligned} \quad (4.22a)$$

$$\frac{\partial X(t, x)}{\partial t} = \mu_x(t, x) \cdot X(t, x) \quad (4.22b)$$

$$\frac{\partial L(t, x)}{\partial t} = \mu_L(t, x) \cdot X(t, x) \quad (4.22c)$$

$$\frac{\partial S(t, x)}{\partial t} = -\frac{1}{Y_S^X} \mu_x(t, x) \cdot X(t, x) - \frac{1}{Y_S^L} \mu_L(t, x) \cdot X(t, x) \quad (4.22d)$$

$$\frac{\partial N(t, x)}{\partial t} = -\frac{1}{Y_N^X} \cdot \mu_x(t, x) \cdot X(t, x) \quad (4.22e)$$

$$\frac{\partial I(t, x)}{\partial x} = k_1 \cdot I(t, x) + k_2 \cdot X(t, x) \quad (4.22f)$$

$$\mu_x = f(S, N, I, t, x) \quad (4.22g)$$

$$\mu_L = f(S, N, I, t, x) \quad (4.22h)$$

$$0 \leq \mu_x(t, x) \leq \mu_{x,max} \quad (4.22i)$$

$$0 \leq \mu_L(t, x) \leq q_{L,max} \quad (4.22j)$$

$$y_{m,L,0} \leq y_m(t_0, x) \leq y_{m,U,0} \quad (4.22k)$$

$$N(t_f, x_0) \leq 0.01 \quad (4.22l)$$

$$S(t_f, x_0) \leq 0.1 \quad (4.22m)$$

$$L(t_0, x_0) \leq X(t_0, x_0) \quad (4.22n)$$

$$L(t_f, x) \geq 0.1 \quad (4.22o)$$

Ammonium chloride salt is used as a nitrogen source during cultivation. It was found that the calculated salt concentration and the theoretical results in the literature were inconsistent when the problem was solved without an upper limit constraint at the final moment. Including this constraint in the model provides more robust and realistic results, as salt concentration is strongly influenced by factors such as the pH of the environment [103]. In addition, the reason for adding a constraint at the final time point for the substrate is to ensure that there is no excess of unused reactant in the cultivation medium.

Dynamic optimization with Partial Differential Algebraic Equations(PDAEs) is very challenging because the direct use of off-the-shelf deterministic optimization solvers is prohibitive and there are additional issues concerning the numerical stability, the robustness of the underlying numerical solver, and computational resources required to handle large-scale problems [44], [104]–[106]. Discretization methods are commonly employed to convert dynamic optimization problems to algebraic optimization problems (e.g., nonlinear program, NLP) [107], [108]. In this study, we use the Pyomo.dae, an open-source Python-based modeling framework, to discretize the PDAE system using finite differences method on the time and spatial domains [44], [94], [95]. The resulting large-scale NLP is then deterministically solved with the Interior Point Optimizer (IPOPT) to retrieve the optimal solution. Next, we extend this analysis to stochastic optimization to study the effect of uncertain elements in algae cultivation and bioreactor optimization.

4.2.3. Stochastic Optimization with Scenario Analysis

Although in the previous sections, we built a very comprehensive two-dimensional isothermal bioreactor model for algae cultivation and addressed its optimization within a dynamic framework using discretization, the system will still be subject to different kinds of uncertainties in the real world. Therefore, it is important to understand and quantify these effects on the system response and overall lipid productivity. To this end, we represent uncertain events for inhibition (K_{il}) and saturation (K_I) constants, k_1 and k_2 constants that represent the location-dependent light intensity, and factors influencing growth, including maximum biomass growth rate ($\mu_{x,max}$) and maximum lipid growth rate ($q_{L,max}$), with scenarios.

The likely scenarios were constructed by assuming a normal distribution with the standard deviation set to 5% of the parameter values. To generate these scenarios, upper and lower bounds were set by either a 5% decrease or increase in the actual parameter values. A set of 30 parameter values was selected from this distribution for the generation of a set of likely scenarios. The same standard deviation is also used to generate unlikely scenarios. These unlikely scenarios were constructed by selecting 15 different parameter values from two separate ranges of values. These ranges were set

at 15% - 5% below and 5% - 15% above the actual parameter values to explore a wider range of the parameters for unlikely scenarios.

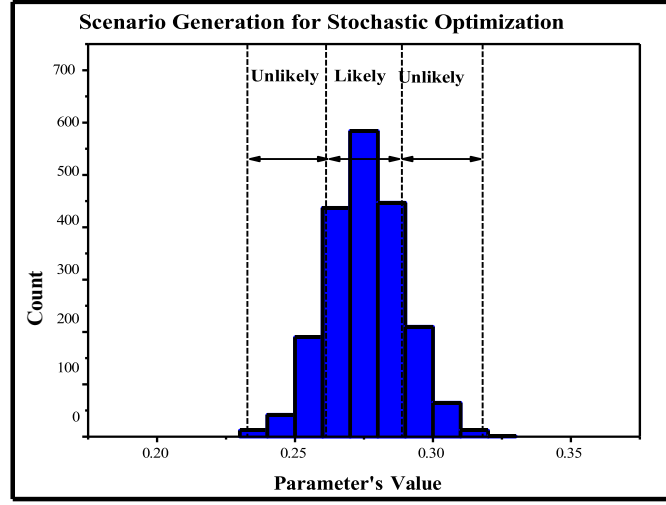


Figure 4.1: Scenario generation for stochastic model.

Finally, the deterministic optimization model in Equation 4.22a-o is modified to account for the scenarios as follows:

$$\max_{S,N,L,X,I} \left(\frac{1}{S_t} \left(\sum_{s=1}^{S=S_t} \frac{L(t_f, x_0, s) - L(t_0, x_0, s)}{t_f - t_0} \right) \right) \quad (4.23a)$$

subject to:

$$\frac{\partial X(t, x, s)}{\partial t} = \mu_x(t, x, s) \cdot X(t, x, s) \quad (4.23b)$$

$$\frac{\partial L(t, x, s)}{\partial t} = \mu_L(t, x, s) \cdot X(t, x, s) \quad (4.23c)$$

$$\frac{\partial S(t, x, s)}{\partial t} = -\frac{1}{Y_S^X} \mu_x(t, x, s) \cdot X(t, x, s) - \frac{1}{Y_S^L} \mu_L(t, x, s) \cdot X(t, x, s) \quad (4.23d)$$

$$\frac{\partial N(t, x, s)}{\partial t} = -\frac{1}{Y_N^X} \cdot \mu_x(t, x, s) \cdot X(t, x, s) \quad (4.23e)$$

$$\frac{\partial I(t, x, s)}{\partial x} = k_1(s) \cdot I(t, x, s) + k_2(s) \cdot X(t, x, s) \quad (4.23f)$$

$$\mu_x = f(S, N, I, t, x, s) \quad (4.23g)$$

$$\mu_L = f(S, N, I, t, x, s) \quad (4.23h)$$

$$0 \leq \mu_x(t, x, s) \leq \mu_{x,max}(s) \quad (4.23i)$$

$$0 \leq \mu_L(t, x, s) \leq q_{L,max}(s) \quad (4.23j)$$

$$y_{m,L,0} \leq y_i(t_0, x) \leq y_{m,U,0} \quad (4.23k)$$

$$N(t_f, x_0, s) \leq 0.2 \quad (4.23l)$$

$$S(t_f, x_0, s) \leq 0.3 \quad (4.23m)$$

$$L(t_0, x_0, s) \leq X(t_0, x_0, s) \quad (4.23n)$$

$$\frac{L(t_f, x, s)}{X(t_f, x, s)} \geq LBR, \quad LBR \in \{0.50, 0.75\} \quad (4.23o)$$

where s is the scenario number and s_t is the total scenario number in the model. The total stochastic lipid productivity is maximized across all scenarios with equal probability subject to the constraints. Given the parameters obtained for each scenario, the restriction of the nitrogen and substrate concentrations at the final time point to a narrower range leads to infeasible simulation results. To overcome this problem, the constraints have been relaxed, and a wider range has been used. In addition, the ratio of lipid to biomass is added as a constraint to increase the minimum product efficiency and quality achieved. For likely and unlikely cases, four simulations were performed with a low lipid biomass ratio (LBR_L) and high lipid biomass ratio (LBR_H), which are 0.50 and 0.75, respectively.

4.3. Results

In this section, several optimization tasks have been carried out for both deterministic and stochastic cases. All computations were performed using an Intel Core i7 processor and 32 GB of RAM, which delivered results in less than 3 minutes in all cases. Proposed equations are implemented through Python/Pyomo programming language for the interface to the IPOPT solver.

4.3.1. Deterministic Optimization

This case employs a dynamic optimization problem where no uncertainty is introduced to model parameters under additional constraints. The resulting operating conditions are provided in **Table 4.4**.

Table 4.4: Deterministic optimization results.

		Variable	Value
Concentrations	Initial	Biomass (g/L)	0.0050
		Substrate (g/L)	2.5035
		Lipid (g/L)	0.0042
		Nitrogen (g/L)	0.0348
	Average	Biomass (g/L)	0.1820
		Substrate (g/L)	0.0902
		Lipid (g/L)	0.1137
	Final Time	Nitrogen (g/L)	0.0002
		Biomass (g/L)	0.1818
	Minimum	Lipid (g/L)	0.1132
		Biomass (g/L)	0.1824
	Maximum	Lipid (g/L)	0.1143
Light	Surface ($\mu\text{mole}/\text{m}^2.\text{s}$)		105.1555
	Final Time Average ($\mu\text{mole}/\text{m}^2.\text{s}$)		94.4513
	Minimum ($\mu\text{mole}/\text{m}^2.\text{s}$)		84.3758
	Maximum ($\mu\text{mole}/\text{m}^2.\text{s}$)		105.1550
	Lipid Productivity		13.0900

An 11.18% increase is obtained in lipid productivity compared to the reference study [23] based on dynamic optimization on fixed parameter values. To favor productivity, an increased amount of substrate and reduced amount of nitrogen is introduced initially under lower light intensity with a reduction of 23.11% at the surface. Thus, a significant reduction in electricity consumption is obtained. However, since the model includes the impact of the depth and the absorption due to chemical compounds, such a light intensity provides sufficient growth capability at spatial coordinates with a relatively manageable product gradient throughout the reactor as shown in **Figure 4.2**.

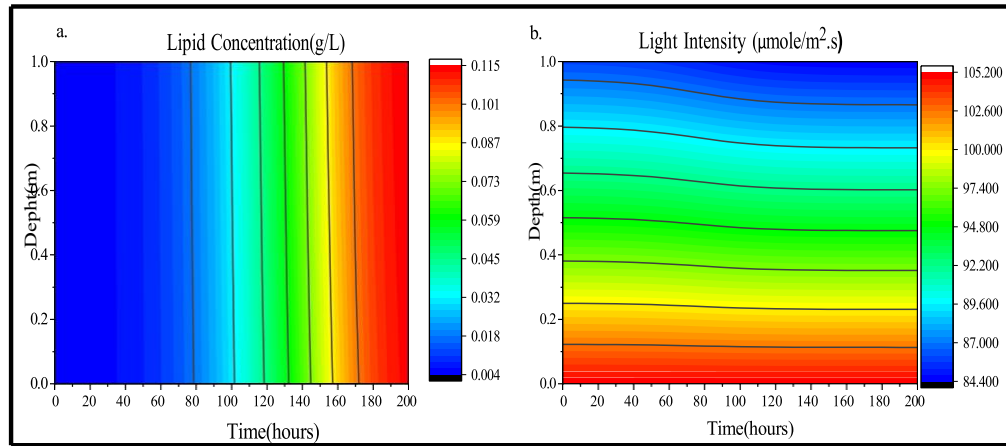


Figure 4.2: Spatial and temporal distribution of some variables a. lipid concentration profile b. light intensity profile.

Despite a higher concentration at the surface all the time, lipid concentration keeps increasing in all spatial coordinates with relatively manageable changes with respect to reactor height, supporting the light sufficiency throughout the reactor as shown in **Figure 4.2.a**. This profile is obtained upon a light intensity profile in **Figure 4.2.b.**, in which the light intensity at the bottom decreases over time due to absorbance/reflectance of biomass and lipid. Average compound profiles are provided in **Figure 4.3**.

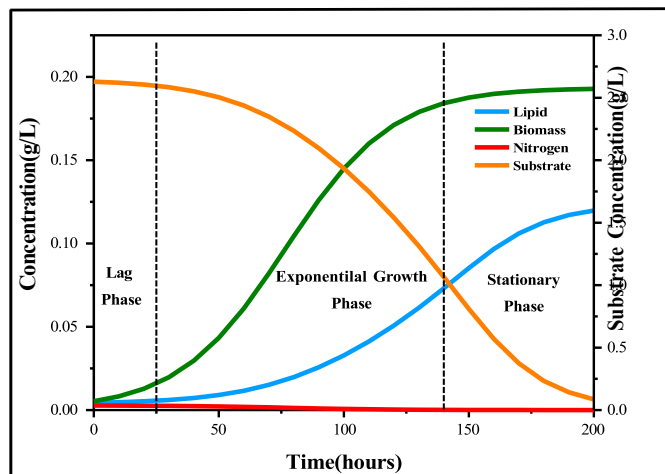


Figure 4.3: Dynamic profile of compounds.

Algae culture does not show a significant amount of cell division and biomass increase in the first 25 hours of the process. This can be explained by the process of adaptation of the algae cells to the growth medium, light, ambient temperature, and pH [109]. This phase is referred to as the lag phase. A significant accumulation of biomass and

lipids was observed in the algae between the 25th and the 140th hour, where nutrient consumption is also significant during the exponential or log growth phase. **Figure 4.3** shows the stationary phase between hours 140 and 200, where the growth rate approaches zero. In this phase, the rate of growth is limited by the fact that one of the nutrients is almost exhausted. Furthermore, even though biomass accumulation has stopped, the cell continues to produce and store products such as lipids or starch [41].

4.3.2. Stochastic Optimization

4.3.2.1. Stochastic Optimization based on Likely Parameter Range

Thirty randomly generated sets of parameters (see Section 4.2.3) are introduced in the optimization problem to ensure the minimum LBR, a measure of typical desirable product distribution at the final time, despite uncertainty in the model parameters which in turn might deliver off-spec production. The lipid fraction in the product might be an important concern in terms of subsequent separation tasks or a particular product to be obtained from further processing of the ultimate mixture. Thus, an additional constraint would introduce a significant impact on initial conditions as well as operation conditions to favor selectivity between biomass and lipid towards the desired regime under the parameter set that defines the uncertainty regime. The optimization results for two different LBRs are provided in **Table 4.5** and **Table 4.6**.

Table 4.5: Results of likely case studies.

		Variable	LBRL	LBR _H
Concentrations	Initial	Biomass (g/L)	0.0090	0.0090
		Substrate (g/L)	2.5475	1.8524
		Lipid (g/L)	0.0089	0.0090
		Nitrogen (g/L)	0.0292	0.0197
	Average	Biomass (g/L)	0.1507	0.1009
		Substrate (g/L)	0.2876	0.2962
		Lipid (g/L)	0.1113	0.0779
		Nitrogen (g/L)	0.0002	0.0007
	Final Time	Biomass (g/L)	0.1443	0.0958
		Lipid (g/L)	0.1106	0.0774
	Maximum	Biomass (g/L)	0.1582	0.1040
		Lipid (g/L)	0.1119	0.0787

Table 4.6: Results of likely case studies (continue).

Light	Surface ($\mu\text{mole}/\text{m}^2\text{s}$)	98.4733	101.3224
	Final Time Average ($\mu\text{mole}/\text{m}^2\text{s}$)	80.9279	83.7957
	Minimum ($\mu\text{mole}/\text{m}^2\text{s}$)	80.2934	82.9257
	Maximum ($\mu\text{mole}/\text{m}^2\text{s}$)	81.6042	84.4268
	Lipid Productivity	13.3608	9.7672

Note that two optimization problems that employ different LBRs in the constraint include average lipid production in the objective function. However, compared to the reference [23], introducing an LBR_L delivered a 13.47% increased lipid productivity whereas an LBR_H reduced productivity by 20.52% compared to the former. Thus, favoring high selectivity among biomass and lipid in the product generates some tradeoff once the average lipid production is concerned. Also, LBR_H constraint causes less consumption of nitrogen and substrate with lower biomass production although initially they are in lower amounts. A higher light intensity provides on the surface to compensate for the reduced nutrient concentrations and promote conversion. Those modifications result in a decrease in both biomass and lipid production, from which the former is more sensitive to those changes; therefore, the LBR_H constraint can be satisfied in each scenario.

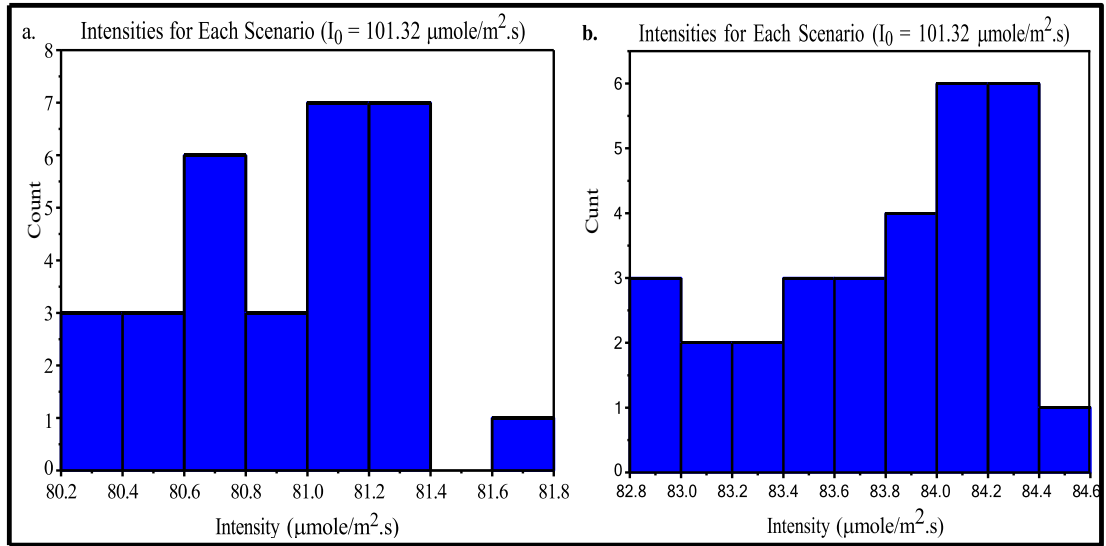
**Figure 4.4:** Light intensity histograms for likely scenarios a. LBR_L . b. LBR_H .

Figure 4.4 shows histogram of light intensities at a closer point to the bottom of the reactor ($x = 0.1$) due to parameter uncertainty. The light intensity varies between $80.29 \mu\text{mole}/\text{m}^2\text{s}$ and $81.60 \mu\text{mole}/\text{m}^2\text{s}$ when an LBR_L is desired, whereas, for LBR_H this range is between $82.93 \mu\text{mole}/\text{m}^2\text{s}$ and $84.43 \mu\text{mole}/\text{m}^2\text{s}$. However, high intensities in **Figure 4.4** are not the sole indicator or driving force in lipid productivity which is

also function of many other impacts including saturation and inhibition constants. **Figure 4.5** shows biomass profiles at different reactor depths and LBRs based on different model parameter scenarios which are utilized in a model with fixed operating conditions.

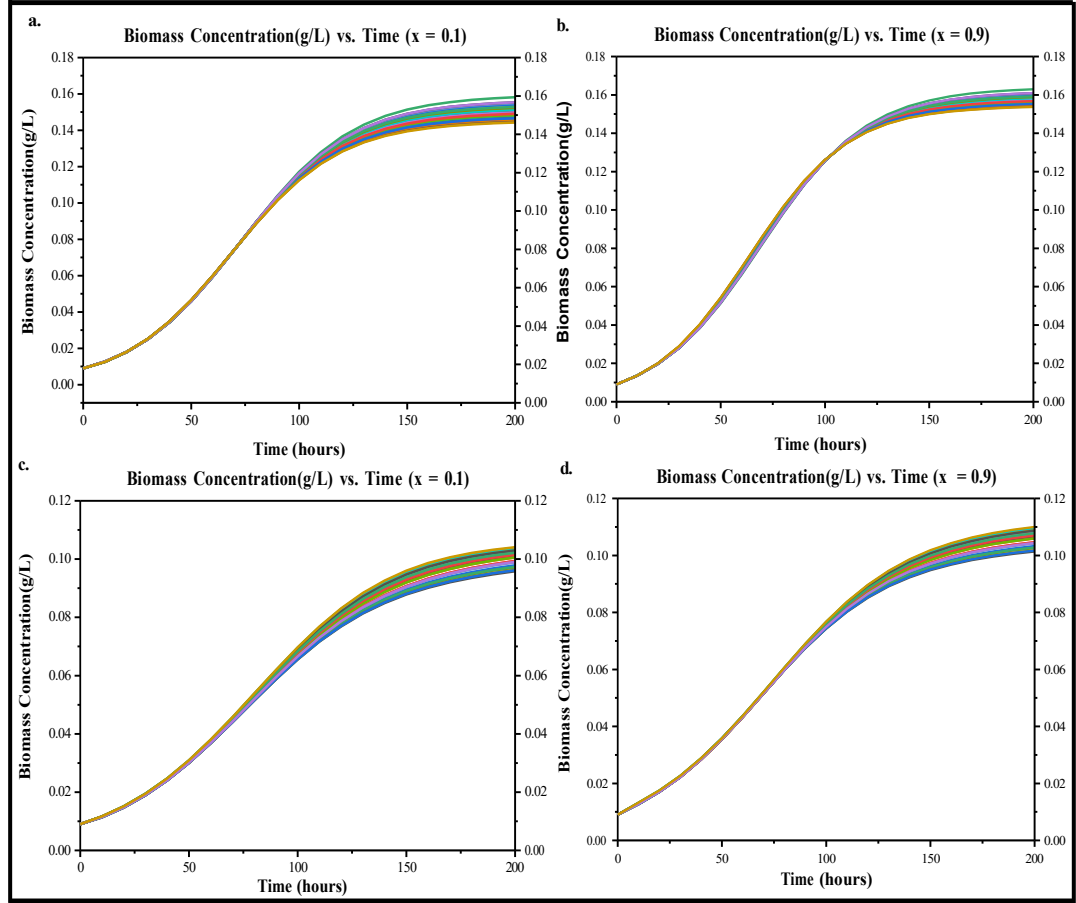


Figure 4.5: Biomass concentration profiles in likely scenarios a. LBR_L and $x = 0.1$ b. LBR_L and $x = 0.9$. c. LBR_H and $x = 0.1$. d. LBR_H and $x = 0.9$.

Figure 4.5 shows that model uncertainty has a more pronounced effect at the depth of the reactor. The range of biomass concentration variability end of the process at a point close to the bottom ($x = 0.1$) is wider than at a point close to the reactor surface ($x = 0.9$). The extent of uncertainty at a particular depth is governed by the propagation of uncertainty which is a function of a high number of contributors including light penetration and growth-related variables. Such variation in the product amounts is also influenced by the operating conditions, besides model parameters, which might be

needed for LBR_H . **Figure 4.5.d.**, compared to **Figure 4.5.b.**, suffers from more relative uncertainty despite having a similar range

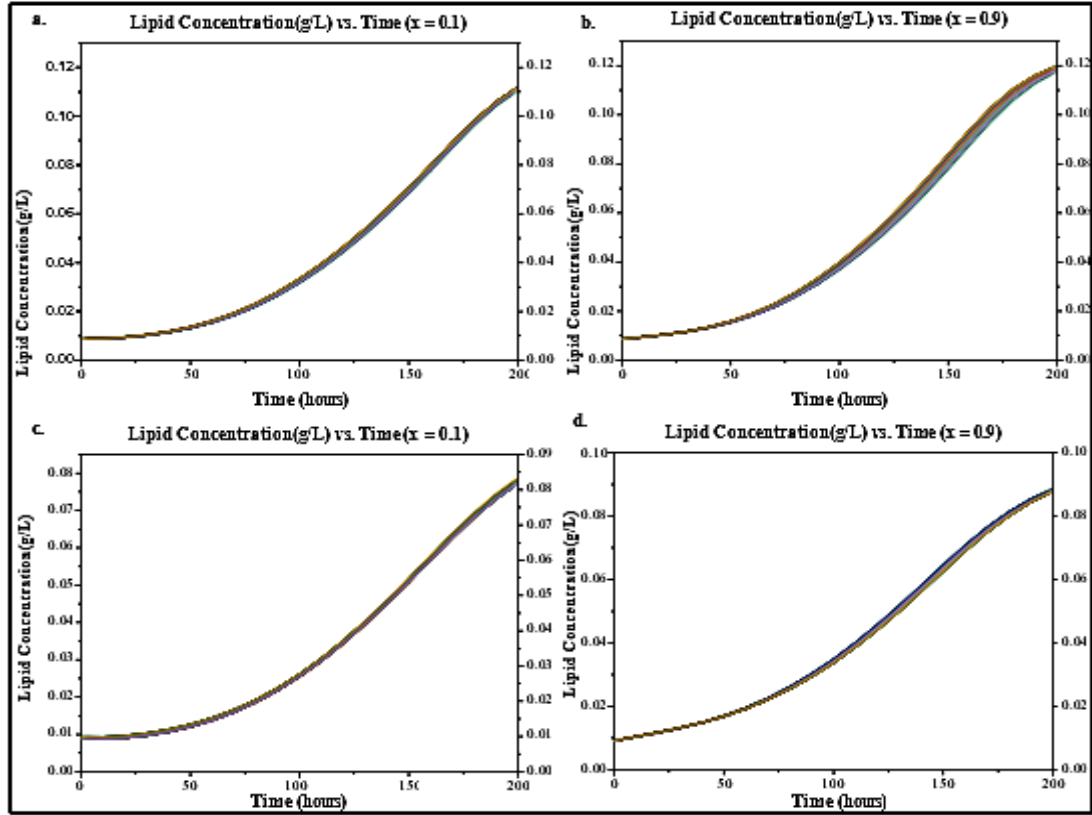


Figure 4.6: Lipid concentration profiles in likely scenarios a. LBR_L and $x = 0.1$ b. LBR_L and $x = 0.9$. c. LBR_H and $x = 0.1$. d. LBR_H and $x = 0.9$.

Figure 4.6. represents dynamic behavior for lipid concentration. Unlike biomass, model parameter uncertainty does not have a significant impact on lipid production under current operating conditions. Note that, model variables do not have to be exposed to uncertainty equally since each of them is constrained by different expressions including different parameters from different nominal values.

4.3.2.2. Stochastic Optimization based on Unlikely Parameter Range

A similar optimization problem is solved based on the unlikely parameter set (see Section 4.2.3). The results of the optimization problem under two different LBR constraints are provided in **Table 4**.

Table 4.7: Results of unlikely case studies.

Variable			LBR = 0.5	LBR = 0.75	
Concentrations	Initial	Average	Biomass (g/L)	0.0090	0.0090
			Substrate (g/L)	2.3990	1.2088
			Lipid (g/L)	0.0089	0.0090
			Nitrogen (g/L)	0.0307	0.0132
		Minimum	Biomass (g/L)	0.1657	0.0614
			Substrate (g/L)	0.1074	0.2845
			Lipid (g/L)	0.1133	0.0511
			Nitrogen (g/L)	0.0002	0.0015
	Final Time	Maximum	Biomass (g/L)	0.1625	0.0545
			Lipid (g/L)	0.1053	0.0503
			Biomass (g/L)	0.1662	0.0676
			Lipid (g/L)	0.1165	0.0525
Light	Surface ($\mu\text{mole}/\text{m}^2\text{s}$)		97.3586	99.4909	
	Final Time Average ($\mu\text{mole}/\text{m}^2\text{s}$)		79.8771	82.4425	
	Minimum ($\mu\text{mole}/\text{m}^2\text{s}$)		78.1716	80.2453	
	Maximum ($\mu\text{mole}/\text{m}^2\text{s}$)		91.9358	84.1879	
	Lipid Productivity		12.6629	5.7842	

The lipid productivity drops significantly compared to the likely case although an LBR_H constraint reduces the lipid productivity in all cases. In addition, the concentrations of nitrogen and substrate that are fed are drastically different. Alongside low nutrient concentrations, there is some increase in surface illumination. The amount of unconsumed nutrients is higher, although less product is obtained for LBR_H . The average light intensity of 30 scenarios near the bottom of the reactor has relatively similar values, despite the significantly different amount of product produced in LBR_L and LBR_H cases as shown in **Figure 4.7**.

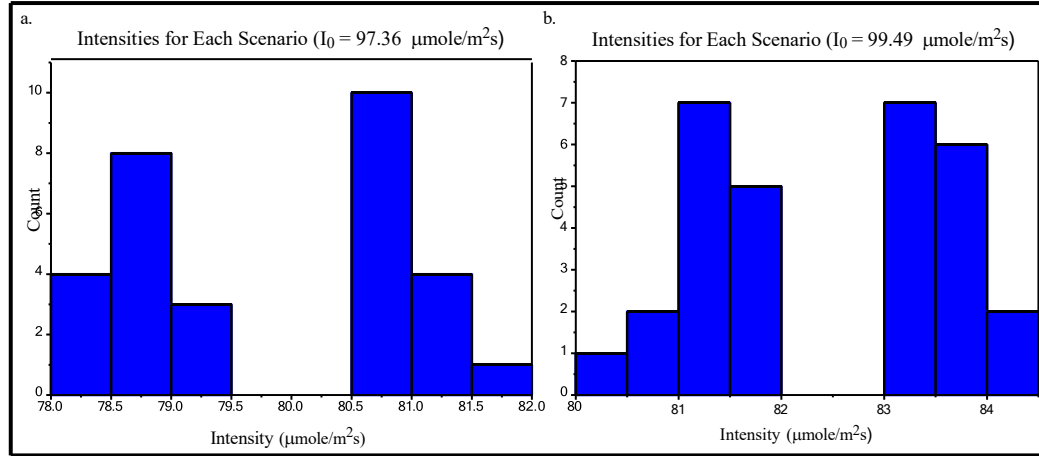


Figure 4.7: Light intensity histograms for unlikely scenarios a. LBR_L . b. LBR_H .

The light intensities in **Figure 4.7.a.** and **Figure 4.7.b.** are concentrated in two ends of the intensity uncertainty range compatible with the scenario generation for the unlikely case. Moving towards the reactor surface, the difference between these groups gradually decreases. This difference can be expressed in terms of the effect of the medium density and parameter uncertainties on the system behavior.

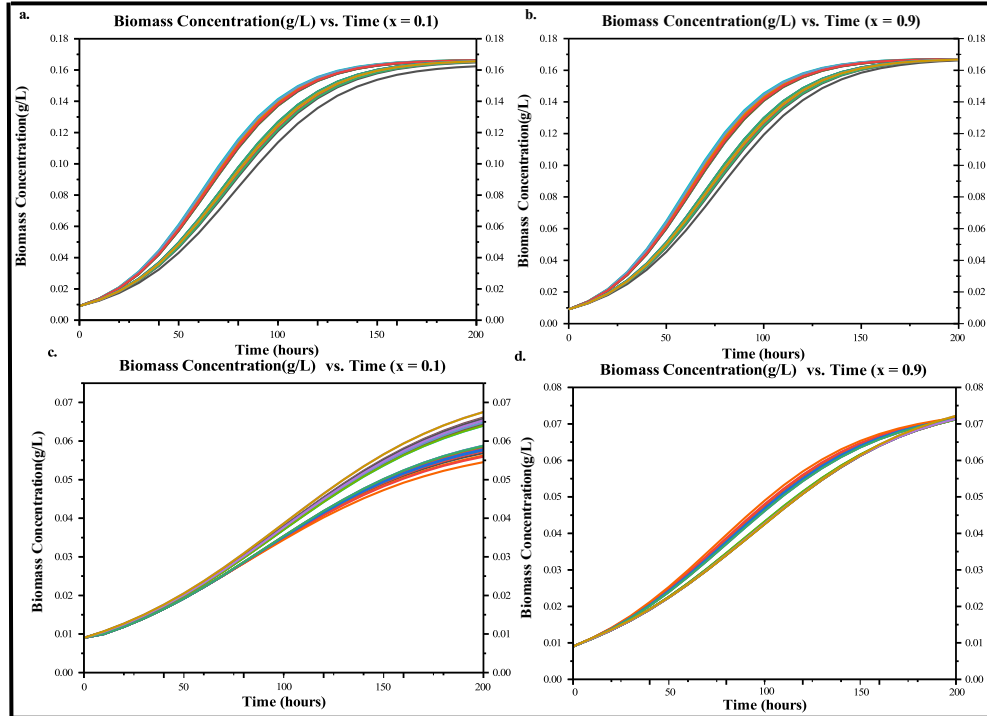


Figure 4.8: Biomass concentration profiles in unlikely scenarios a. LBR_L and $x = 0.1$ b. LBR_L and $x = 0.9$. c. LBR_H and $x = 0.1$. d. LBR_H and $x = 0.9$.

Figure 4.8.a. and **Figure 4.8.b.** show the results of the LBR_L scenarios and **Figure 4.8.c.** and **Figure 4.8.d.** show the simulation results of the LBR_H scenarios, respectively. For the LBR_L case, the depth does not have a significant impact on the biomass dynamic profile. However, a relatively wider range of distribution is observed at the bottom of the reactor over time. The effect of the constraint defined in the model between two simulation results at the same location is clearly observed in **Figures 4.8.a.** and **4.8.c.** or **4.8.b.** and **4.8.d.**, respectively. Furthermore, the lipid concentration profiles from this study are presented as follows:

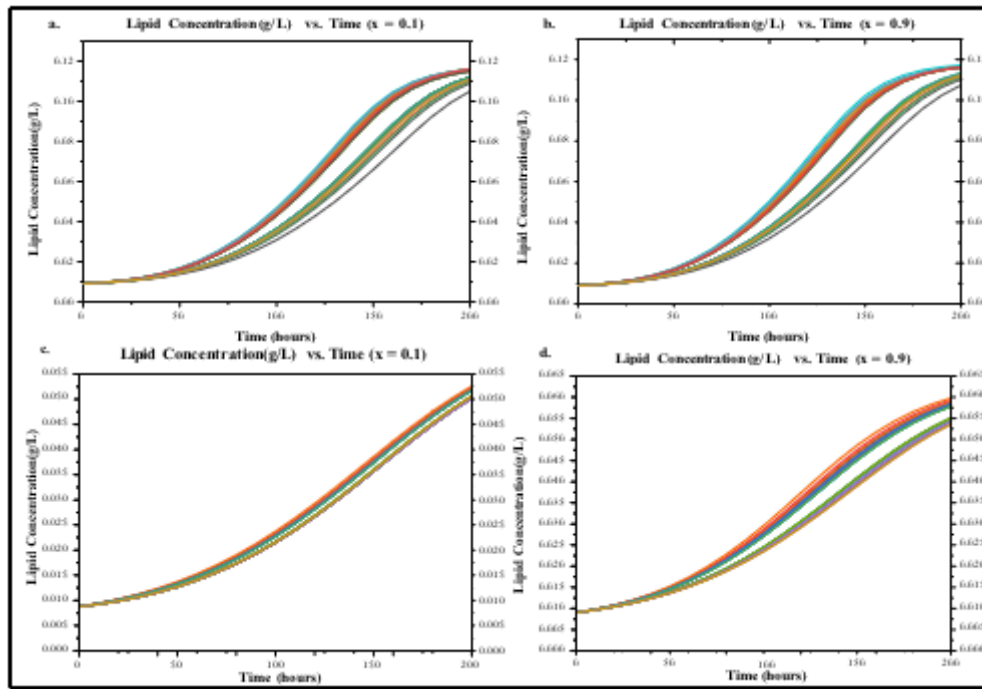


Figure 4.9: Lipid concentration profiles in unlikely scenarios a. LBR_L and $x = 0.1$ b. LBR_L and $x = 0.9$. c. LBR_H and $x = 0.1$. d. LBR_H and $x = 0.9$.

Figure 4.9. shows the dynamic lipid profile at LBR_L and LBR_H optimization tasks. The former suffers from a larger amount of uncertainty which is mostly independent of depth. In contrast, the surface dynamic profile exhibits more variation once the LBR_H constraint is implemented.

4.4. Conclusion

This study focuses on the development of deterministic and stochastic approaches to microalgae cultivation processes design and operation. To this end, the problem is transformed into two dimensions and optimized deterministically by adding the location (depth) dimension to the dynamic formulation, unlike traditional methods. By adding the depth dimension to the dynamic formulation, the problem is modified and optimized deterministically, creating a more flexible and realistic model that is more sensitive to dynamic conditions and produces consistent results. Lipid productivity increased by 11.18% from 11.775 mg/L.d to 13.090 mg/L.d when comparing the results of dynamic and deterministic optimization compared to the reference study. The minimum amounts of initial substrate, nitrogen, and minimum light concentration to be supplied from the surface were also calculated while maximizing the lipid concentration. In comparison to the theoretical result, an efficient system with higher lipid productivity was obtained by using more substrate (acetate) and less nitrogen and light intensity.

A stochastic nature was introduced through uncertainty to the model parameters, which are included in a two-dimensional model. This helps decision-making processes become more robust under unmodeled or unmeasured impacts during the process. In this study, four stochastic optimization problems are solved to account for scenario likelihood and selectivity requirements. In scenario generation, the studies were carried out by selecting 30 different parameters from certain ranges, under the normal distribution assumption. The product quality at the end of the process was ensured to remain above a certain ratio by adding low and high constraints for the lipid-to-biomass ratio. However, when high selectivity is desired, significant differences in the amount of lipid and biomass obtained were observed and the average lipid productivity declined. Conversely, the average lipid productivity for likely scenarios is higher compared to deterministic simulations when this constraint is set low.

In summary, although deterministic studies are generally carried out in literature, there are some stochastic studies on algae cultivation and biofuel production. These studies include applications such as surrogate model predictions or supply chains. Based on this shortcoming, we constructed a two-dimensional dynamic algal photobioreactor model to measure the effect of light intensity, as well as nitrogen and

phosphorus concentrations in the culture medium, on the lipid productivity of *Chlamydomonas Reinhardtii*. By integrating stochastic programming and spatiotemporal modeling of the bioreactor, our study helps us to understand the uncertain effects of key parameters on lipid productivity and algal growth in a more differentiated and comprehensive way.

5. INTEGRATED STOCHASTIC SCHEDULING AND SUPERSTRUCTURE OPTIMIZATION FOR SHORT-TERM PRODUCTION PLANING

5.1. Introduction

In today's high-volume manufacturing environment, efficient and predictable production is of paramount importance. Companies want to transform their raw materials into valuable products in the shortest time, at the lowest cost and with the least waste [110]. For this purpose, it is extremely important and necessary to carry out short-term scheduling studies. Short-term scheduling (STS) is a process expressed in mathematical equations used to plan and manage a company's daily or a few days production [111]. This process involves planning within a certain period of time in a way that will be most efficient and profitable, with minimal loss of existing resources [111]. During this planning, considering the amount of product demanded by the consumer and the current process conditions, the order of the process operations and where they will be positioned in the selected time period is determined by considering mathematical and physical constraints. Given these constraints, detailed planning results in a safe and efficient production schedule.

The challenge of short-term scheduling in a petrochemical plant is one of the most significant tasks in the field. Various production planning software has been developed for this purpose. The two most widely used of these software's are RPMS (Refinery and Petrochemical Modelling System) and PIMS (Process Industry Modelling System), developed by Honeywell and ASPEN Tech which are commercial software [112]. In addition to the aforementioned software, engineers engaged in process optimization and planning have also developed their own models to facilitate the creation of production plans. These models are structured according to three primary categories, corresponding to the processes observed in a refinery [113]. The initial category encompasses the unloading, mixing, and transportation of raw materials or oil from carrier tankers. The second category encompasses the storage of raw materials and their subsequent processing and conversion into products. In this section, optimal production planning is achieved by considering the physical parameters and production costs of the process elements, including the reactor, pump and compressor

etc., production capacity, processing time, and product impurity. In the final stage of the refinery, the blending process is conducted to ensure that the produced product meets customer demand, and the resulting product is shipped [112], [113].

The reactor part, due to the nature of chemical science, involves solving variables such as reaction kinetics expressions, component concentration changes, and reactor operation mode (isothermal, non-isothermal, etc.) by restricting mathematical expressions with ordinary differential equations or partial differential equations if solved in more than one dimension [113]. However, solving this problem mathematically requires a significant amount of effort. In order to reduce the mathematical processing load required to solve this problem, it can be overcome by linearizing the equations or using new equations with linear programming. Although linear programming models and algorithms provide an optimum solution in production planning in the refinery, inaccuracies caused by non-rigorous linear models can affect the forecast performance and the profit and quality achieved [114]. In this direction, complex and dynamic processes are planned by developing non-linear short-term scheduling models. This planning methodology offers a means of significantly overcoming the disadvantages of linear models.

The literature contains numerous examples of short-term planning studies that employ linear and non-linear programming models. [115] developed a mathematical model to represent the supply chain in an oil refinery. This model comprises a highly complex structure comprising a refinery, terminal, and pipelines. In this study, a large-scale MINLP model was created using flow rate and properties, production variables, and storage-related variables as decision variables. The model performance was tested using different scenarios. [116] is a study on the planning of mixing processes that directly affect product quality in the petrochemical plant. The mixing process creates a model with a very complex and non-linear structure. In this model, the McCormick relaxation method and normalized multiparametric decomposition technique are employed to identify the global optimum solution. This approach enables the creation of convex relaxations, thereby reducing the computational load. The developed model was evaluated in comparison with studies in literature, with regard to both the results and the solution speed. In contrast to traditional models, the model developed by [117] does not focus solely on the input and output flows of the units. Furthermore, the model was developed to provide more accurate results by developing a non-linear model that also includes process variables. The proposed planning model consists of two different

nonlinear models for the distillation tower and one nonlinear model for the remainder of the refinery. This model is a non-linear type of model due to the constraints that meet the requirements for mass balances, process efficiency, and product quality. The study resulted in enhanced product quality and efficiency, as well as more robust and realistic results, by overcoming the limitations of linear models.

Another crucial aspect of short-term process scheduling is the inherent uncertainty in the processes themselves [118]. MINLP models are typically based on precise parameter values, but it is widely acknowledged that these values can fluctuate in the real world for a multitude of reasons. To illustrate, the geopolitical location of the facility where production will be carried out can give rise to a multitude of uncertainties in product supply chains due to factors such as political and military tensions in the surrounding area. Furthermore, unforeseen circumstances, such as the global pandemic of 2020, have resulted in disruptions to supply chains and production planning [119]. It has been observed that such uncertainties may lead to disruptions or even complete cessation of production processes. Consequently, STS optimization problems that consider uncertainty in parameter values are of paramount importance. In their study, [120] developed a stochastic chance-constrained model for the optimization of the crude oil processing process. This model differs from traditional approaches in that it encompasses the stages of the three-stage refinery planning previously discussed. The model comprises the following steps: crude oil unloading and mixing (Phase 1), separation process (Phase 2), and transfer of the produced product and inventory control (Phase 3). The portion of the study that addresses uncertainty is the crude oil purification units with continuous and discrete joint probability distributions. To reduce the computational burden, the model was tested with case studies for its applicability by transforming it into equivalent stochastic chance-constrained mixed integer linear programming. Similarly, [121] classify a petrochemical refinery under three spatial concepts: discharging and mixing, production and delivery. The proposed model was tested with case studies for short-term planning studies, and it was found to be sufficient for its applicability in realistically large problems. In another study, [110] conducted a study considering the uncertainties in the quality of crude oil feeds during refinery planning. In this study, a stochastic model was created by considering the effect of crude oil quality on refinery profitability and purchasing decisions. In order to determine the quality of the raw

material, uncertainty is included in the model by using true boiling point (TBP) curves. The resulting structure ensures that the best raw material selection is made, and appropriate planning results are obtained. This study is the first academic study to stochastically apply refinery and crude oil selection, considering TBP curves, under crude oil uncertainty.

In today's context, it is of paramount importance to align the designs of process systems with regulations and requirements, as well as to renew them with new technologies, to minimize their environmental impact and associated costs. In addition, it is possible to select appropriate equipment from within the existing complex structure using superstructure optimization, considering the existing processes' ability to respond to changing demands in a timely manner and with minimal production costs. From this point forward, the most appropriate production plan can be devised by taking into account the amount of need and production costs in short-term planning. This method allows for a quick response to changes in demand while minimizing production costs. As a result, the efficiency of the process increases, and a competitive advantage can be gained. For instance, [122] developed an integer linear programming model for superstructure optimization in the process synthesis of a biofuel plant aiming to produce microalgae-based biofuel. The model enabled the identification of a process structure that minimized production costs and met the production target. Furthermore, in a section of the article, short-term production planning optimization was conducted within the model by imposing time constraints as a case study. Following the completion of the case studies, the minimum biodiesel cost was determined to be between \$6.4/L and \$8.53/L.

This study develops an original model for short-term planning of mixing, reaction, and separation units in a production facility. The model is designed to align with the requirements of a small number of academic research and production planning in the industry. Unlike traditional planning models, the developed model combines stochastic and superstructure optimization. This integration aims to achieve maximum profit with minimum equipment use and therefore minimum production cost under variable conditions. This innovative approach plays an important role in the production of products that will meet consumers. Furthermore, the incorporation of uncertainty into the model affords the planning process greater flexibility, thereby enhancing the reliability of the resulting outcomes. From a broader perspective, the deployment of a

minimal number of process equipment throughout the entire complex process network confers several advantages, including sustainability and the effective utilization of natural resources.

5.2. Model Formulation

This study presents the development of a 24-hour refinery planning model, which incorporates adjustments and additions to the Short Term Scheduling model developed by [123]. The constraints employed in this model can be classified into the following categories: allocation, capacity, material balance, duration, sequence, timing constraint, minimum product constraint, cost constraints and equipment selection constraints.

5.2.1. Allocation Constraint

An allocation constraint is a constraint that specifies that only one event can occur at any given event point. At this point, if the value of the binary variable $yv(j, n)$ is equal to 1, then one of the mixing reactions or separation processes occurs at the time point “ n ” in the process unit “ j ”. Furthermore, the binary variable $wv(i, n)$ represents the start time of the process operation, with “ i ” denoting the specific steps occurring within the process. In this study, as it is a basic process structure, only the mixing, reaction, and separation steps are considered [123].

$$\sum_{i \in I_j} wv(i, n) = yv(j, n) \quad \forall j \in J, n \in N \quad (5.1)$$

5.2.2. Capacity Constraint

The capacity constraint represents the minimum and maximum feasible throughput of the selected process unit. In this expression, V_{ij}^{min} represents the minimum capacity volume; $b_j(j_1)$ is the binary variable that allows selection from the complex superstructure; $B(i, j, n)$ represents the production volume of the “ i ” process step in

the

$$V_{ij}^{min} \cdot wv(i, n) \cdot b_j(j_1) \leq B(i, j, n) \leq V_{ij}^{max} \cdot wv(i, n) \cdot b_j(j_1) \quad (5.2) \quad "j"$$

unit at time “ n ”; V^{max} represents the maximum production capacity [124].

$$\forall i \in I, j \in J_i, j_1 \in J_1, n \in N$$

5.2.3. Stream Capacity Constraint

The flow capacity limit represents a physical constraint that expresses the maximum flow rate between process units. In equation 5.3, $ST(s, n)$ represents the flow rate of mass flow “ s ” at event point “ n ”. $ST(s)^{max}$ signifies the maximum flow rate between the selected process units.

$$ST(s, n) \leq ST(s)^{max} \cdot b_j(j_i), \forall s \in S, n \in N, i = \{1, 2, 3\} \quad (5.3)$$

5.2.4. Material Balance Constraint

The mass balance constraint is a mathematical expression that represents the net change in material within a given set of process units. This expression can be further simplified to the following form:

$$Input - Output + Generation - Consumption = Accumulation$$

In characterizing this expression for any mass flow, it can be seen that the amount of product or raw material at the time “ n ” is $ST(s, n)$, the amount of flow at the time “ $n - 1$ ” is $ST(s, n - 1)$, and the final product produced, $d(s, n)$, depending on the type of flow, can be written as an equation that depends on the amount of product produced or consumed. In this mathematical expression, the coefficients ρ_{si}^p and ρ_{si}^c are dependent on the amount of production and consumption, respectively [121], [123], [124].

$$\begin{aligned}
ST(s, n) = & ST(s, n - 1) - d(s, n) \\
& + \sum_{i \in I_s} \rho_{si}^p \sum_{j \in J_i} B(i, j, n - 1) + \sum_{i \in I_s} \rho_{si}^c \sum_{j \in J_i} B(i, j, n)
\end{aligned} \tag{5.4}$$

$$\forall s \in S, j \in J_i, n \in N$$

5.2.5. Sequence Constraints (Same Task in Same Unit)

The initial constraint within the sequence determines that the commencement of any process step is contingent upon the completion of the preceding job. In this context, the term “ H ” refers to the total planning time. When both variables $wv(i, n)$ and $yv(j, n)$ are equal to 1, the constraint is reduced to the following: $T^s(i, j, n + 1) \geq T^f(i, j, n)$, which implies that the job at event time $n + 1$ cannot commence prior to the completion of the job at event time n . This satisfies the sequential rule. In the event that the values of these binary variables are equal to zero, the constraint will be rendered ineffective. Given that “ H ” will be a relatively large number, $T^s(i, j, n + 1)$ can assume any positive value, rendering the constraint ineffective in this case.

$$T^s(i, j, n + 1) \geq T^f(i, j, n) - H \cdot (2 - wv(i, n) - yv(j, n)) \tag{5.6a}$$

$$\forall i \in I, j \in J_i, n \in N \text{ and } n \neq N$$

$$T^s(i, j, n + 1) \geq T^s(i, j, n) \tag{5.6b}$$

$$\forall i \in I, j \in J_i, n \in N \text{ and } n \neq N$$

$$T^f(i, j, n + 1) \geq T^f(i, j, n) \tag{5.6c}$$

$$\forall i \in I, j \in J_i, n \in N \text{ and } n \neq N$$

$$T^s(i, j, n + 1) \geq T^f(i, j, n) \tag{5.6d}$$

$$\forall i \in I, j \in J_i, n \in N \text{ } i = 1, 2, 3$$

The second constraint states that for any given process unit, the beginning of each new period “ $n + 1$ ” must occur at a point later than the beginning of the previous period “ n ”. Similarly, a comparable expression is employed for completion times in another constraint.

The final constraint guarantees that a process phase in a process unit cannot commence

prior to the conclusion of the preceding phase. Collectively, these constraints guarantee that the work progresses in a sequential, consistent and uninterrupted manner, thereby ensuring the orderly and efficient management of the workflow [123], [124].

5.2.6. Sequence Constraints (Different Task in Different Unit)

This constraint enables the scheduling of disparate jobs within disparate units in a sequential manner. Binary variables (wv and yv) regulate the efficacy of the constraint under specific conditions, compelling the jobs to be completed in a prescribed sequence. Given that “ H ” is a considerable number, the constraint becomes ineffectual in certain instances, thereby affording greater flexibility. However, when both binary variables assume the value of 1, the constraint becomes operational, compelling the jobs to be completed in a specific sequence and with continuity.

$$T^s(i, j, n + 1) \geq T^f(i', j', n) - H \cdot (2 - wv(i', n) - yv(j', n)) \quad (5.7)$$

$$\forall i \in I, i' \in I_j, j, j' \in J_i, n \in N \text{ and } i \neq i', n \neq N$$

5.2.7. Sequence Constraints (Completion of Previous Tasks)

This constraint takes into account the completion time of jobs to ensure that jobs are performed in a certain order and continuity. It requires that a job starting in a certain period be adjusted according to the completion time of all related jobs in previous periods. In this way, a logical sequence is achieved between jobs and all related jobs are completed before starting in any period.

$$T^s(i, j, n + 1) \geq \sum_{n' \in N, n' \leq n} \sum_{i' \in I_j} (T^f(i', j, n') - T^s(j, n')) \quad (5.8)$$

$$\forall i \in I, j \in J_i, n \in N, n \neq N$$

5.2.8. Time Horizon Constraints

These constraints restrict the production stages to be completed within the specified production time. Consequently, the operational periods of the production units commence and conclude within a 24-hour timeframe.

$$T^f(i, j, n) \leq H, \forall i \in I, j \in J_i, n \in N \quad (5.9a)$$

$$T^s(i, j, n) \leq H, \forall i \in I, j \in J_i, n \in N \quad (5.9b)$$

5.2.9. Minimum Amount of Product

Equation 5.10 states that the total amount of final product to be obtained from the separation units should not be less than 500 tons per day. The minimum amount of products produced will be 500 tons. This constraint is an effective mathematical inequality in the selection of process equipment and the calculation of working times.

$$\sum_{n \in N} B(3, j_3, n) \geq 500 \quad n \in N \quad (5.10)$$

5.2.10. Mixer Cost Estimation

The mathematical expression demonstrates the financial implications of the raw material mixing process for the company. In the equation, $C^{mix}(j, sc)$ represents the cost of each mixing equipment “j” in all scenarios (sc). On the other side of the equation, $p_{m,cons}$ represents the construction cost; $p_{m,maint}$ represents the maintenance cost; $p_{m,energy}$ represents the energy cost and $p_{m,eff}$ represents the energy efficiency of each mixer.

$$\begin{aligned}
C^{mix}(j, sc) = & \sum_{n \in N} [(T^f(1, j, n) - T^s(1, j, n)) \cdot (B(1, j, n))] \\
& \cdot (p_{m,cons}(1, j, sc) + p_{m,maint}(1, j, sc) \\
& + (p_{m,energy}(1, j, sc) \cdot (2 - p_{m,eff}(1, j, sc)))) \\
& \forall j \in J_1, n \in N, sc \in Sc
\end{aligned} \tag{5.11}$$

5.2.11. Reactor Cost Estimation

The cost of the selected reaction units is calculated using Equation 5.12. In the equation, $p_{r,lab}$ is the labor cost; $p_{r,cons}$ is the construction cost per ton and hour depending on the construction material and other features of the reactor; $p_{r,fuel}$ is the fuel cost used during heating or cooling for the efficient realization of the reaction; $p_{r,cat}$ is the catalyst cost depending on the amount and type of catalyst used; and $p_{r,util}$ is all other services required during the conversion of raw materials into products.

$$\begin{aligned}
C^{reac}(j, sc) = & (\sum_{n \in N} [(T^f(2, j, n) - T^s(2, j, n)) \cdot (B(2, j, n))] \\
& \cdot (p_{r,lab}(2, j, sc) + p_{r,cons}(2, j, sc) + p_{r,fuel}(2, j, sc) \\
& + p_{r,cat}(2, j, sc) + p_{r,util}(2, j, sc))) \\
& \forall j \in J_2, n \in N, sc \in Sc
\end{aligned} \tag{5.12}$$

5.2.12. Separator Cost Estimation

The separation cost per unit time and per ton is calculated using Equation 5.13. In this equation, $p_{s,solvent}$ represents the cost of the solvent used; $p_{s,constr}$ represents the construction cost of the separation units; $p_{r,utility}$ represents all auxiliary services to the process; $p_{s,eff}$ represents the process efficiency.

$$\begin{aligned}
C^{sep}(j, sc) = & \left(\sum_{n \in N} [(T^f(3, j, n) - T^s(3, j, n)) \cdot (B(3, j, n))] \right. \\
& \cdot (p_{s,solvent}(3, j, sc) + p_{s,constr}(3, j, sc) \\
& \left. + p_{r,utility}(3, j, sc) \cdot (2 - p_{s,eff}(3, j, sc))) \right) \\
& \forall j \in J_3, n \in N, sc \in Sc
\end{aligned} \tag{5.13}$$

5.2.13. Selection Constraints

The application of the constraints set forth in Equations 5.14-5.16 as superstructure optimization constraints allows for the identification of the most suitable combination of four mixers, three reactors, and three separation units, given the constraints. The application of these constraints allows for the calculation of the most suitable 10 unit combinations from a total of 26 process equipment.

$$\sum_{n=1}^{10} b_{mixer}(j) = 4 \quad \forall j \in J_1 \tag{5.14}$$

$$\sum_{n=1}^8 b_{react}(j) = 3 \quad \forall j \in J_2 \tag{5.15}$$

$$\sum_{n=1}^8 b_{sep}(j) = 3 \quad \forall j \in J_3 \tag{5.16}$$

5.2.14. Objective Function

The objective function is to minimize the cost of the entire process.

$$\min_{wv, yv, B, d, ST, T_s, T_f, b_m} C^{mix}(j_1, sc) + C^{react}(j_2, sc) + C^{sep}(j_3, sc) \tag{5.17}$$

The optimization problem model can be summarized as follows:

$\min$ *Objective Function* (5.17)

subject to:

Allocation Constraint (5.1)

Sequence Constraints (5.6 – 5.8)

Capacity Constraint (5.2)

Time Horizon Constraints (5.9)

Stream Capacity Constraint (5.3)

Minimum Amount of Product (5.10)

Material Balance Constraint (5.4)

Selection Constraints (5.14 – 5.16)

Duration Constraint (5.5)

The optimization superstructure model can also be summarized as follows:

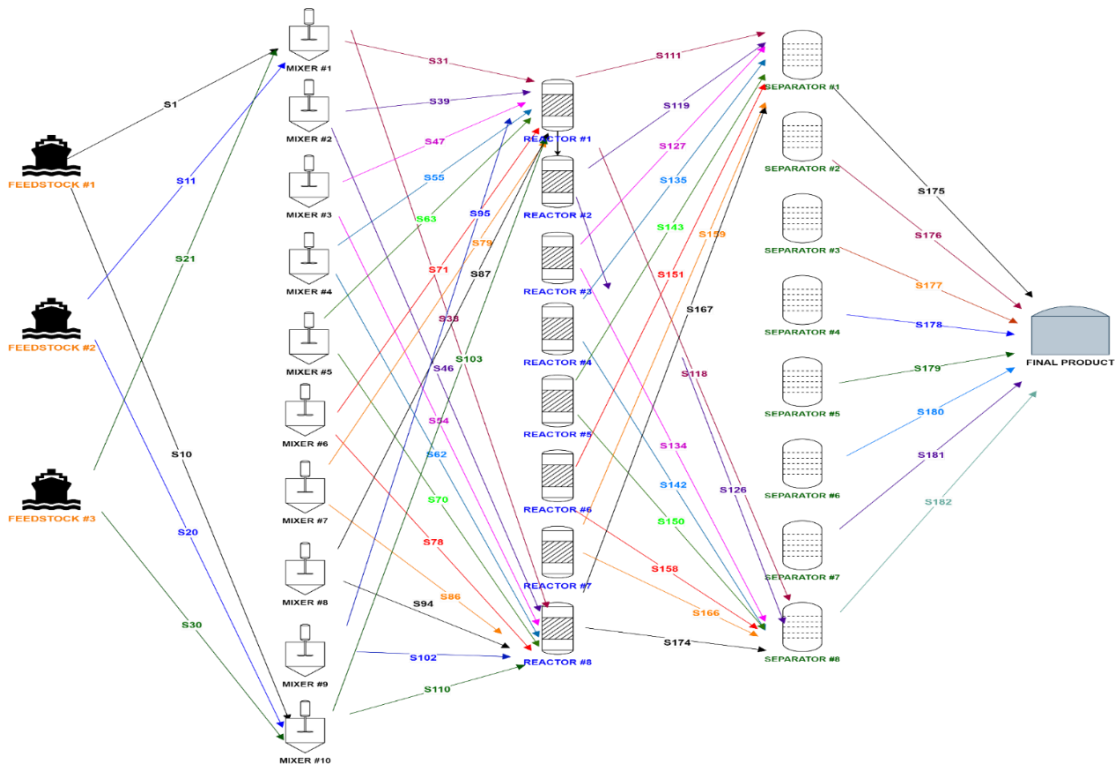


Figure 5.1: Superstructure of the problem.

Figure 5.1 illustrates the process by which raw materials from three distinct sources are combined in four of ten mixers to create an intermediate product. This mixture is then transformed into a product mixture containing impurities by selecting three of eight reactors. The purification of this mixture is achieved through the selection of three of eight separation units, after which the final product is stored. The structure encompasses a total of 182 flows, comprising both product and feed.

5.3.Results

In this study, deterministic and stochastic solutions of 24-hour production planning of a production facility consisting of 26 equipment including mixing reaction and separation process units were investigated. All computations were performed using an Intel Core i7 processor and 32 GB of RAM. Proposed equations are implemented through Python/Pyomo programming language for the interface to the GUROBI solver. Modelling was done on the IMPL platform and MILP problems were solved with GUROBI 10.0.3. Nonlinear problems were linearized with IMPL's SLP algorithm and solved using GUROBI Linear Programming [125].

5.3.1. Case 1: Stochastic Scheduling

In this case study, random values were assigned to process and cost parameters using a standard deviation value of $\sigma = 0.5$, and a 24-hour production plan was created with minimum cost by selecting random values for each scenario. The creation and selection of parameter values are as follows:

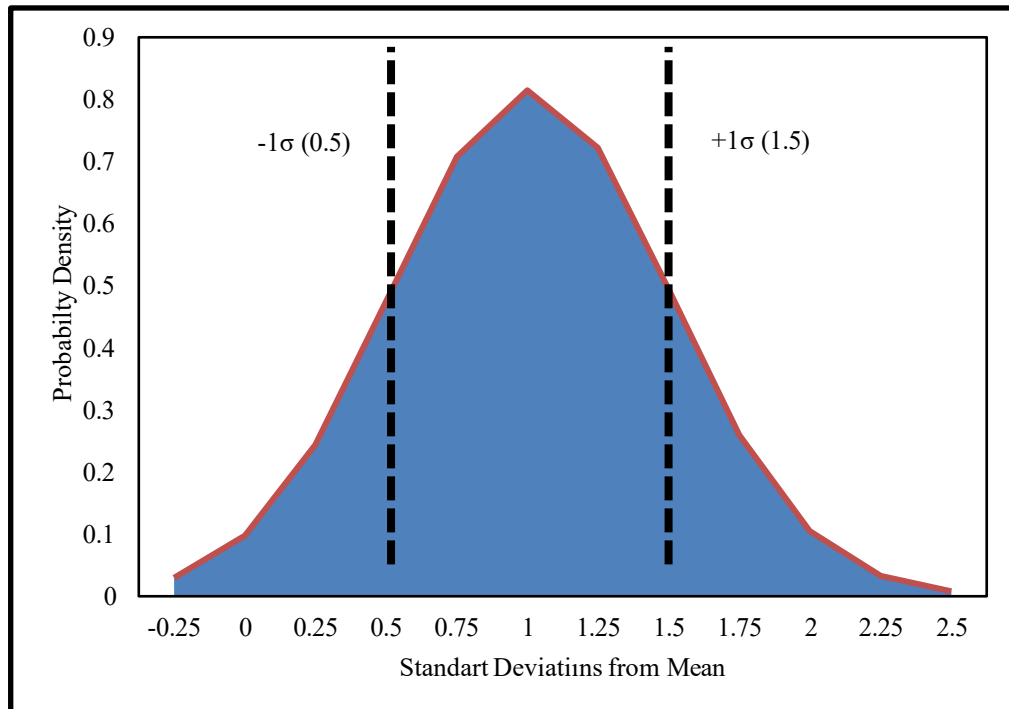


Figure 5.2: Parameter generation with $\mu = 1$ and $\sigma = \pm 0.5$.

After solving the model, the cost distribution for each selected equipment and scenario is as follows:

Table 5.1: Cost distribution for each scenario.

ID	Sc. 1	Sc. 2	Sc. 3	Sc. 4	Sc. 5	Sc. 6	Sc. 7	Sc. 8	Sc. 9	Sc. 10
M-2	5849.2	3761.4	3749.1	4228.6	3761.4	4392.9	3557.9	5529.2	5529.2	4392.9
M-3	2787.4	2197.4	3300.3	2197.4	3312.8	3963	3312.8	2937.1	3963	3300.3
M-4	3926.2	5451.6	3501.3	5451.6	3501.3	3941.1	5295.9	3941.1	350	5564.9
M-9	3932.2	4443.5	3212.3	3212.3	4148.3	2848.1	2702.9	4148.3	2130.8	3200.2
R-2	8645	4800	4781.1	5542.3	4800	5815.7	4491.1	7942.5	7942.5	5815.7
R-3	13738.7	10434.9	16874.3	10434.9	16954.4	21424	16954.4	14625.6	21424	16874.3
R-5	12464.3	8871.1	18213.6	15124.6	22482.5	11679.9	12433.9	11679.9	18800.8	12483.1
S-1	7365.4	12377.2	9337.6	7729.1	12235.8	7326.5	9772	11179.2	8366.6	10811.2
S-2	16992.2	17332.8	12605.1	17991.1	10231.7	14626.9	16906.4	17837.7	13093.2	13830.5
S-5	10662.4	5527.9	7421.2	9807	7686.4	7640.8	8342.4	6935.2	8230.9	7961
Total Cost	86363	75197.8	82995.9	81718.9	89114.6	83658.9	83769.7	86755.8	89831	84234.1

Out of 10 available mixers, Mixers 2, 3, 4, and 9 were selected as the optimal process units. In terms of process efficiency, Mixer-3 (M-3) had the lowest average mixing efficiency at 0.473, followed by Mixer-10 (0.493) and Mixer-5 (0.503). The highest average efficiencies were observed in Mixer-7 (0.589), Mixer-8 (0.603), and Mixer-1 (0.616). Regarding installation costs, M-3 had the lowest average cost at \$0.835/tons·h, while M-1 had the highest at \$1.087/tons·h. Similarly, M-3 also recorded the lowest maintenance and energy costs at \$0.334/tons·h and \$0.250/tons·h, respectively. In contrast, M-1 had the highest values for both, at \$0.435/tons·h for maintenance and \$0.326/tons·h for energy.

When the economic parameters of Mixer-2 (M-2) are examined, it stands out as a unit with average values across most criteria. However, with its 110 tons processing capacity, it is considered a suitable option for medium- to large-scale production. Despite being less favorable in terms of cost parameters, M-2 offers a simpler and more easily controllable process by enabling the use of a single unit, avoiding the complexity of a multi-unit system that might arise from combining lower-cost, lower-capacity mixers.

M-3 is selected in the model solution due to its lowest operating cost, making it optimal

in terms of satisfying both the objective function and process constraints. Although its efficiency is lower than that of other units, its low energy consumption significantly contributes to its selection by minimizing total energy costs. Moreover, with a high production capacity of 120 tons, M-3 is well-suited for medium- and large-scale production plans, making it a highly viable process unit overall.

Mixer-4 (M-4) has relatively high-cost parameters compared to other mixers, but it offers the second highest production capacity at 140 tons. This makes it highly suitable for large-scale production plans, especially those requiring quick responses or high-volume orders. As shown in **Figure 5.3**, M-4 is the most utilized unit in the production schedule, highlighting its importance. In a short-term production scenario with limited equipment, M-4 plays a critical role by enabling the mixing of large quantities in a single batch, simplifying the overall process structure, reducing production costs, and helping satisfy model constraints.

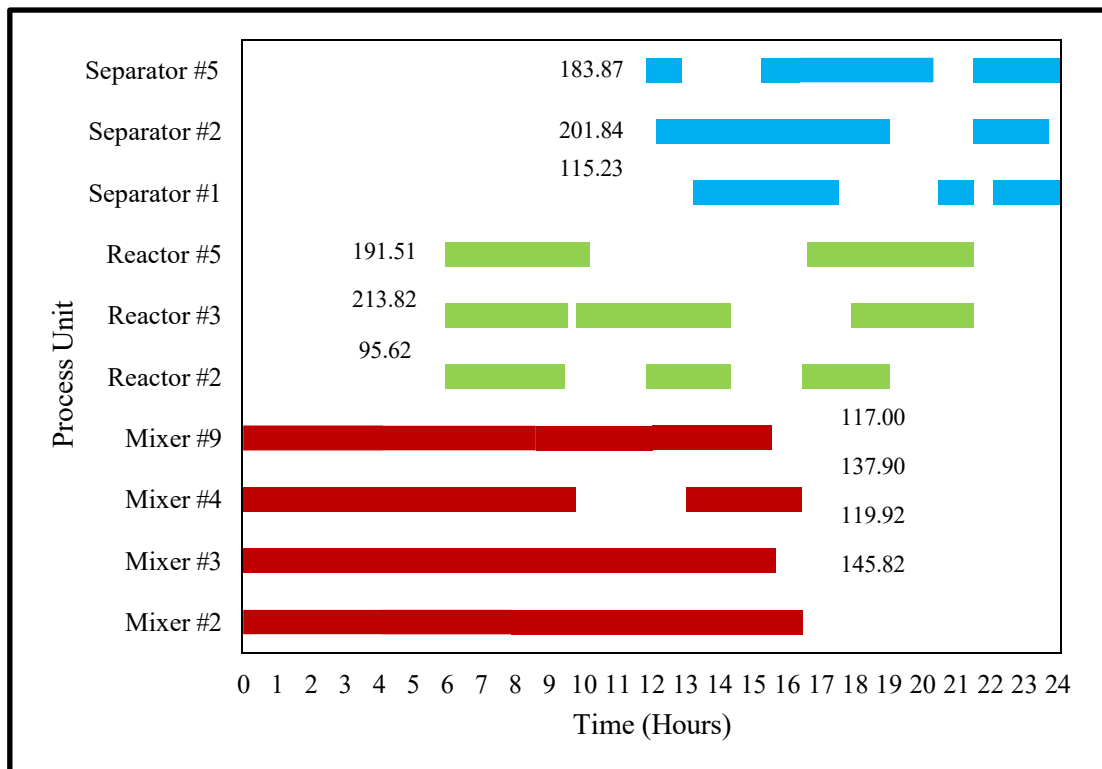


Figure 5.3: Results of stochastic model.

The final selected unit, Mixer-9 (M-9), has the lowest capacity at 60 tons per batch. Despite its smaller size and relatively high energy and maintenance costs, it serves as a supportive unit in the production system. M-9 is particularly useful for small-scale

production runs or when the combined capacity of larger mixers like M-2, M-3, and M-4 are insufficient. As shown in **Figure 5.3**, M-9 operates in parallel with M-3 and M-4, effectively complementing their functions and contributing to the flexibility and efficiency of the production plan.

The model includes a reaction stage where raw materials are converted into the final product after premixing, using one of eight available reactors. Each reactor has distinct production capacities and cost parameters, including labor, construction, fuel (energy), catalyst, and utility costs. The two main criteria for reactor selection in the model are minimizing cost and selecting the fewest number of reactors capable of meeting the required short-term production. Based on these criteria, R-2, R-3 and R-5 are identified as the optimal process units. R-2 has the third-lowest operating cost at an average of \$1.482/tons.h, with reasonable installation and operational expenses. It offers a process capacity of 85 tons and a runtime of approximately 4.26 hours, which is well-suited for short-term planning. Similar to Mixer-9, Reactor-12 (R-12) plays a supportive role in the system. It is used to fulfil remaining production needs when high-capacity reactors are insufficient. This added flexibility enables the model to achieve a simplified production plan with fewer selected units.

Another selected process unit is R-3, chosen primarily for its low operating cost. With a production capacity of 75 tons, R-3 serves as the main reactor for material processing over a 24-hour period. Its production time of 3.99 hours allows it to be assigned to multiple events within the schedule. Considering its efficiency, runtime, and operating cost, R-3 stands out as one of the most stable and sustainable units in the process superstructure.

The final selected reactor is R-5, which has the second-highest production capacity among all reactors. It plays a critical role in achieving short-term production targets. In addition to its physical capacity, R-5 also offers the second-lowest operating cost after R-3. It completes a 110 tons batch in approximately 4.93 hours, enabling it to fulfil a significant portion of the required production in a single cycle. This makes R-5 a highly cost-effective and reliable unit for continuous and target-oriented production.

The last stage of the superstructure, as in all manufacturing systems, involves the removal of unwanted by-products that may affect product quality. For this purpose, the

model includes 8 separation units (S-units), from which only three are to be selected to meet final product requirements. Based on cost, schedule compatibility, and capacity, the model identifies S-1, S-2, and S-5 as the optimal separators.

Separator-1 (S-1) is the most efficient unit in the system, with a separation efficiency of 71%. However, this comes at a high cost S-1 has the highest solvent and utility expenses, at \$2.72/ tons.h and \$3.12/ tons.h respectively, and the highest combined installation and operating cost, averaging \$2.49/tons.h. Despite its relatively small capacity (50 tons), its ability to complete a batch in just 2 hours makes it ideal for urgent or critical production needs. Due to this strategic advantage, the model includes S-1 as one of the three selected separators despite its higher costs.

Separator-2 (S-2) is another unit identified as optimal by the model. Like S-1, it offers high efficiency at 63%, but with more moderate operating costs. With a balanced batch capacity of 60 tons and a process time of 2.2 hours, S-2 serves a supporting role, filling capacity gaps when other units are fully utilized. As seen in **Figure 5.3**, while S-5 is the primary separator, S-2 contributes to production continuity and adds flexibility to the scheduling strategy. Its favorable cost-to-performance ratio makes it a valuable addition to the selected units.

The final selected separator is S-5. Although its efficiency is lower (57%), it has the second-lowest average operating cost at \$2.13/tons.h. With a large batch capacity of 90 tons, S-5 functions as the main separation unit, operating consistently near full capacity. As seen in **Figure 5.3**, S-5 handles the bulk of the separation tasks efficiently, making it the core production unit for this process stage due to its favorable balance of cost, capacity, and throughput time.

5.3.2. Case 2: Deterministic Scheduling

In another case study, the model was solved only in one scenario and a deterministic solution was obtained. In the obtained solution, a superstructure optimization study with a capacity of 500 tons/day was carried out by selecting 4 mixers, 3 reaction and 3 separation units as in Case 1. As a model solution, M-1, M-4, M-6 and M-10 were calculated as optimum mixing units, R-2, R-4 and R-6 as optimum reaction units, and S-2, S-3 and S-5 as optimum separation units. The distribution of construction &

operating costs of the selected process equipment is as follows:

Table 5.2: Cost distribution of each process unit.

ID	Operating Cost	ID	Operating Cost
M-1	2512.9 \$	R-4	10869.9 \$
M-4	3264.8 \$	R-6	15942.7 \$
M-6	8082.6 \$	S-2	9501.2 \$
M-10	3361.5 \$	S-3	13996.4 \$
R-2	7520.9 \$	S-5	6289.0 \$
Total Cost: 81341.9			

The Gantt chart, which expresses the production plan obtained according to the results calculated by the model, is as follows:

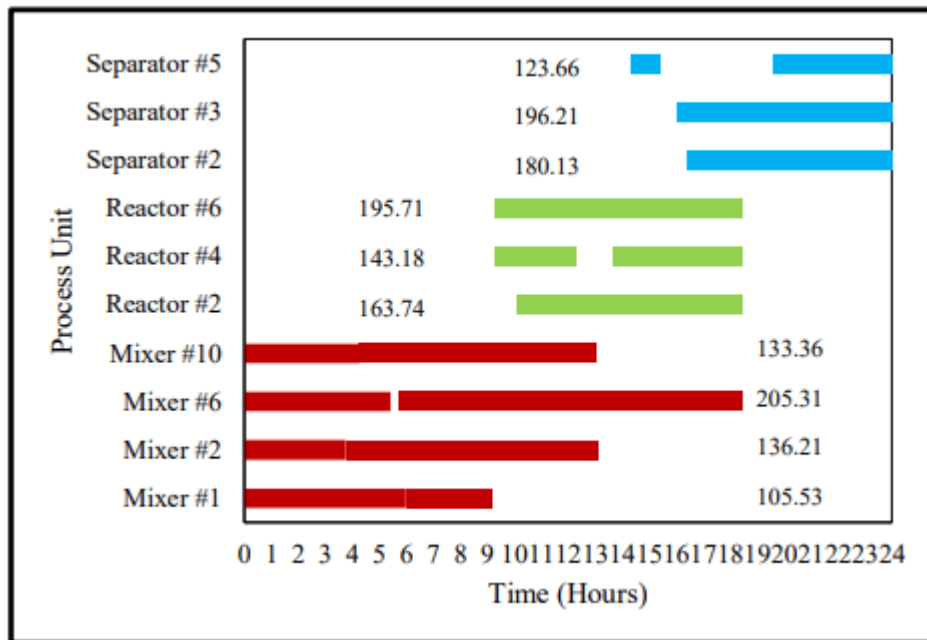


Figure 5.4: STS results for deterministic model.

When the selected mixers are examined, although M-1 has the second lowest efficiency in the superstructure (49.7%), it is calculated as an optimum result in the solution of the model due to its advantageous construction & operating cost. Despite its high production capacity and low cost, M-1 has undertaken approximately 20% of the production. When the other selected mixing units are considered, due to the low efficiency of M-1, the model has used this mixer as a support and complement to manage short-term, low-batch tasks cost-effectively thanks to its low energy consumption and maintenance cost.

M-2 has the lowest efficiency among all mixing equipment, but since its installation

& operating costs are quite low, it has been calculated as an optimum result by the model. The selection of M-2 shows that it attaches importance to the completion of tasks in short-term planning and compliance with the time horizon rather than unit efficiency. This mixer was selected to maintain the continuity of the system in short tasks or critical time periods when other mixers are full. Despite its low efficiency, it played a key role in the production flow thanks to its ability to fill short task intervals.

Although M-6 has high installation & operating costs, it enables large-scale production with its high process capacity. In addition, M-6 has undertaken approximately 41% of the production on its own, allowing for fewer tasks and more easily applicable short-term production planning. M-6 plays an important role in the model in terms of simplifying and implementing the short-term production plan.

When M-10 is examined in terms of efficiency & cost, it is calculated as the optimum element for the process with its economic returns despite its low efficiency. When **Figure 5.4** is examined, it is a process element that can be placed between long-term equipment such as M-6 or short-term equipment such as M-1 and contributes to filling the gaps and undertaking a supporting role in the medium term. Although its low efficiency seems disadvantageous theoretically, its low energy costs make M-10 an attractive candidate instead of units with high efficiency and high energy costs.

When the stochastic solution and the deterministic solution are compared, while the lowest cost superstructure optimization is performed in the deterministic case study where the cost is prioritized for a single scenario, there is a complex superstructure optimization in the stochastic study that provides the lowest cost in multiple scenarios and can meet all constraints simultaneously. For this reason, while the choices in the deterministic case study are more precise and have a wide range, the choices in the stochastic case study are more controlled and have a narrow range. In addition to all this, all cost parameters are fixed and do not vary in the deterministic solution. Considering that cost expenses do not remain fixed due to inflation, exchange rate fluctuations, politics and similar reasons and are constantly fluctuating, the deterministic model is limited in terms of operational flexibility and only makes production planning according to the current cost parameters. In the stochastic solution, operational flexibility is quite high and the ability to adapt in times of crisis or in case of production setbacks is quite high. When evaluated from this perspective, the stochastic solution is a production planning model with quite advantageous returns

in terms of risk management and sustainable production planning.

5.3.3. Case 3: Event Point Number

In the last case study, the effect of the number of event points on the short-term production planning and production cost was examined. In this case study, models were solved with the number of event points being 7, 8, 9 and 10. **Table 5.3** shows the cost obtained in the simulations based on the number of event points, the amount of product obtained and the cost per ton.

Table 5.3: Results for each event point.

Number of Event Point	7	8	9	10
Value of Objective F. (\$)	765387	803050	852615	957743
Amount of Product (tons)	500.86	500.00	500.97	500.08
Mean Cost/tonne for Each Scenario	1528.13	1606.10	1701.94	1915.18

In the simulation performed with 7 event points, since there was a relatively low number of planning rights during planning, production was calculated as planned long time intervals and a large-scale, simplified and block production was planned. When the Gantt chart in **Figure 5.6.a.** is examined, this situation is clearly seen. In the chart, M-2, M-5, M-8, R-3, R-4 and R-7 units share the load of the 24-hour production plan without interruption. Continuing production on the same machines continuously minimizes the factors that will create losses in production such as transitions between machines and the start-up process that will occur during machine transition and allows the efficient evaluation of production time. On the other hand, by continuously choosing advantageous machines in terms of cost, an advantage was also provided in total cost and cost per ton item. As seen in **Figure 5.5** and **Table 5.3**, the most advantageous simulation in terms of cost was obtained in 7 event points. As can be seen, although the 7-event point simulation provides quite sufficient results for a production plan that is as simple as possible and highly efficient, the fact that it can create a relatively limited number of decision work plans makes this simulation weak due to its flexibility and reaction to unusual situations.

When the number of event points increases to 8, although a block production plan continues in the mixing units in the production plan, short-term production plans have

been made in the reaction and separation units compared to the production plans with 7 event points, and there is flexibility in the model's responses to production negatives in this part of the plan. Each process unit used in production (except M-5) has a homogeneous production volume and is calculated as balanced in the production plan. Due to this balanced production amount calculated and the mixing equipment in the middle-upper segment in terms of cost, the production cost has increased slightly and has risen to \$1606.1 per ton. However, considering the disruptions and instant changes experienced in large-scale production facilities, it is quite possible that this cost increase will be subsidized with the ability to act in times of crisis thanks to the system flexibility gained despite the increase in cost.

When the number of event points is increased to 9, the system's ability to respond to crisis scenarios increases considerably, but it also brings with it a few difficulties since an operationally complex structure is obtained. Although block production plans such as the 9-event point production plan continue partially, there is an increase of approximately 33% in the total working time of the mixing units compared to the 8-event point plan. Although there is a partial balance in the production quantities in **Figure 5.6.b.**, there is a significant increase in production costs in **Figure 5.6.c.** due to the more homogeneous production quantities per mixer and the preference of economical process and lower-medium segment process equipment. Although the 9-event point solution has the ability to respond quite strongly to production uncertainties, it is calculated as a relatively high-cost production plan when the cost-efficient balance is considered.

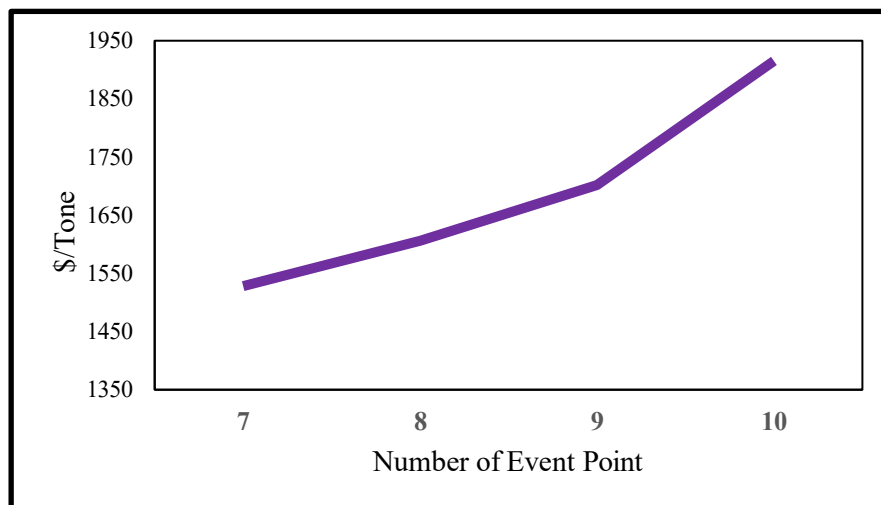


Figure 5.5: Cost / tone for each event point simulation.

Finally, the behavior of the system was examined by increasing the number of event points to 10. In this simulation, the system made a production plan at a level that could minimize the crises and problems that could be experienced in production in the short term, rather than long-term block work plans. Although the created production plan is quite satisfactory for managing crisis moments, the fact that many and short-term irregular productions were made throughout the plan caused the production plan to become quite complicated and caused a serious increase in production costs. It is more meaningful and vital to prefer production plans with such a high number of event points in sectors where there is no stock and production urgency, considering the cost-efficient balance.

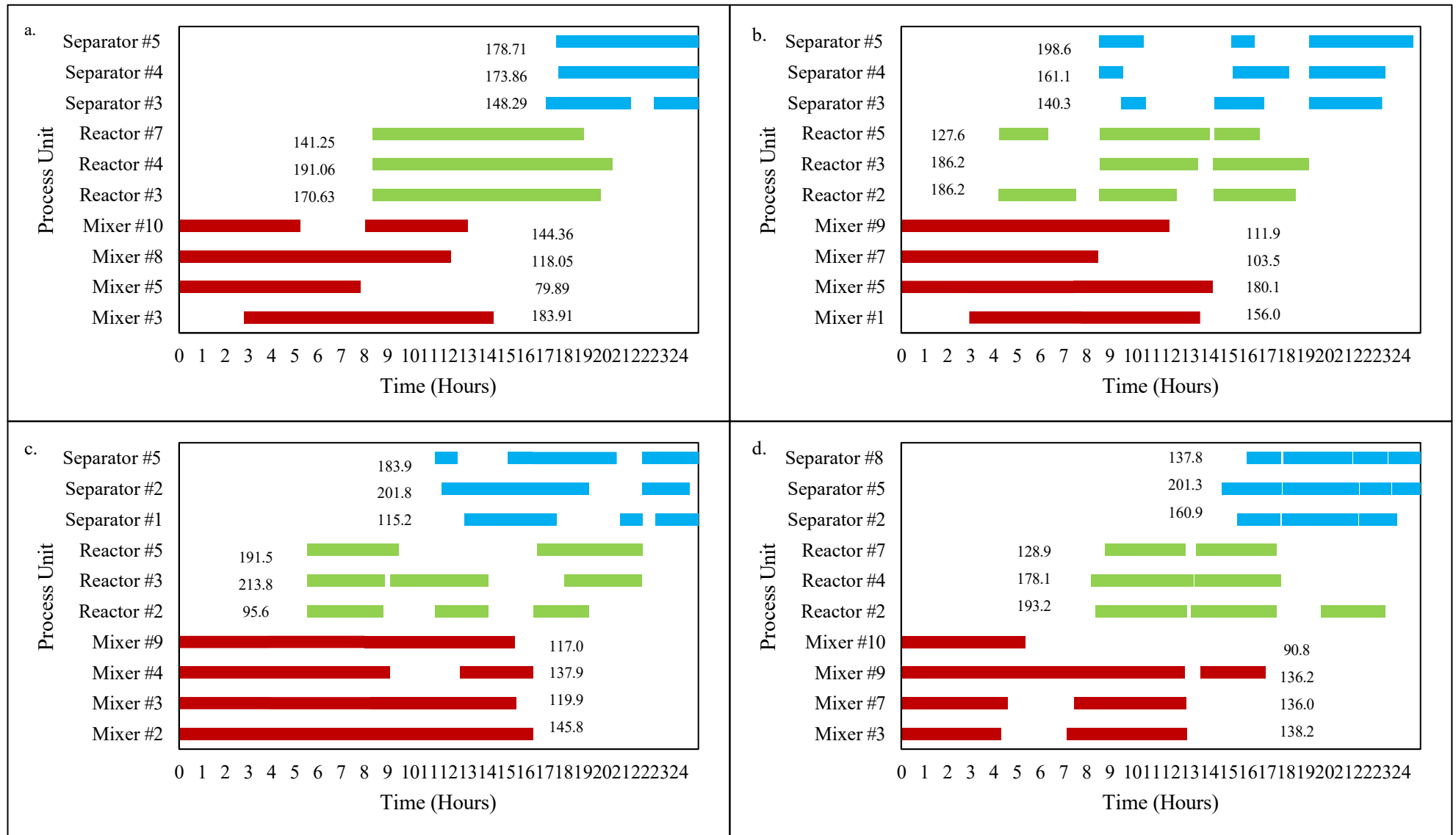


Figure 5.6: STS results for a. 7 event point b. 8 event point c. 9 event point d. 10 event point.

5.4. Conclusion

In today's increasingly industrialized world, achieving maximum efficiency and quality with minimum cost has become one of the most fundamental elements of being competitive in the market. Therefore, using modernized automation systems instead of traditional methods in production is of great importance in terms of effectively evaluating capacity, manpower and raw materials. In parallel with all these developments, making production plans almost flawlessly and with flexibility to respond to instant changes plays a critical role in ensuring efficiency and sustainability in production. In this context, preparing daily production plans not only with traditional methods but also by considering mathematical models and uncertainties will bring many advantages such as uninterrupted production, efficient use of resources and cost savings. For this purpose, a short-term (24-hour) production plan study was carried out by modifying the mathematical models developed by Ierapetritou and Floudas.

Although this study includes the physical and temporal constraints of traditional planning models, it aims to provide solutions to the problems that large-scale production facilities frequently encounter in daily life, such as exchange rate fluctuations, sudden changes in prices, and disruptions in raw material supply. In this direction, in the model developed using randomly generated cost parameters, it is aimed to provide all model constraints simultaneously with the minimum cost objective function. In this respect, the study offers an innovative approach. In addition, another important difference of the model is that short-term stochastic production planning is synthesized with superstructure optimization. In this way, it has become possible to select or calculate the most suitable process elements for the purpose from the complex structure, and thus a strategic production plan has been created that will provide maximum efficiency with minimum cost.

In this study, models were developed to provide optimum production planning through three different case studies. In the first case study, stochastic modelling, uncertainties were defined with 10 samples selected from 1000 randomly generated data with cost parameters $\sigma = \pm 0.5$. Accordingly, an appropriate production plan was created by determining the most suitable 4 mixers, 3 reactors and 3 separation units that simultaneously provide all constraints and objective functions of the model. The

stochastic solution provided management of uncertainties under multiple scenarios and provided more balanced resource utilization. Although the costs obtained in the solution of this model seem higher compared to the deterministic solution, it provides quite flexible and sustainable results thanks to the ability to take quick action in times of crisis, the efficient use of all resources and the optimization of the superstructure. The second case study, the deterministic model which is an approach suitable for production facilities with more stable economic conditions and a fixed supply chain. This model enables production with minimum cost and enables simpler planning of long-term and high-volume production through block production. However, it has significant limitations in terms of decision-making ability and flexibility in times of crisis. In the last case study, the effect of the number of "event points" on the production plan was examined. This analysis provides a very comprehensive and satisfactory simulation in terms of evaluating the relationship between the flexibility of production plans and the superstructure synthesis under all physical and economic conditions. It was observed that parallel to the increase in the number of event points, production plans transitioned from a block structure to a fragmented structure and production costs increased. In summary, the most important difference of this study is that, unlike traditional planning methods, the superstructure optimization of the production facility and short-term stochastic production planning are carried out simultaneously. In this way, it becomes possible to create efficient, simplified and sustainable production plans by considering economic uncertainties and physical constraint.

6. CONCLUSION

In this thesis, the biological, physical and economic dimensions of the microalgae cultivation process, which is one of the promising and highly potential renewable energy sources, are addressed with a holistic approach, and mathematical models that enable the design of sustainable productions are created and their optimization is aimed. For this purpose, these models developed are enriched with not only deterministic solutions but also stochastic uncertainties, providing flexibility in the solution capabilities of the model and providing a robust decision-making mechanism. In this context, in the second part of the study, a complex mathematical model containing nonlinear ordinary differential equations that mathematically express microalgae cultivation is developed. In the developed model, the effects of basic process parameters such as light color (wavelength), initial concentration, feed stream purity, dilution coefficient and cultivation medium type on biomass concentration are analyzed. In this way, it has played an active role in the calculation of optimum process conditions that provide maximum biomass concentration and maximum profitability. In the model, parameter estimation was made via MATLAB with the help of experimental data in the literature, and then optimum solutions were obtained using the BONMIN solver in the Pyomo library. With the help of the obtained solutions, process parameters and production strategies that ensure the most profitable maximum biomass concentration were calculated.

In the third part of the thesis, a stochastic structure was obtained by integrating uncertainty into the economic parameters of the model, and cost-oriented scenario analyses were conducted in biomass production to determine optimum process conditions. With the help of the calculated optimum dilution coefficient, optimum reactor volume and sizing were also calculated. As a result of these analyses, it was shown that the system can show high performance even under uncertainty, and therefore offers an optimization structure with high applicability in production systems even under variable cost conditions.

In the third part, instead of classical ODE (Ordinary Differential Equations) models, a time and depth-dependent PDAE (Partial Differential Algebraic Equations) model was developed, reflecting more realistic process dynamics. With this model, the changes in light intensity depending on the depth of the medium, the effects of nitrogen and

substrate concentrations depending on time and depth were modeled with precision, and multidimensional optimization of lipid and biomass production processes was achieved. The findings obtained in this section revealed that microalgae exhibit very complex interactions with parameters such as light intensity, nitrogen and substrate, and that stochastic models provide more reliable outputs compared to deterministic models. In the fourth section of the thesis, an innovative model was developed for 24-hour short-term production planning on an industrial scale, including process unit selection, workload distribution and timing optimization. The model has a unique structure that combines superstructure optimization with stochastic production planning. Thanks to this structure, sustainable production strategies that provide efficient use of resources even under variable market conditions were proposed. In three separate case studies; it was shown that the deterministic approach is suitable in stable and fixed conditions, but the stochastic approach, which provides flexibility in times of crisis, offers more strategic outputs. In addition, it has been observed that by increasing the number of event points used in production planning, the plans become more fragmented and flexible, but the costs increase accordingly. In line with all these analyses, the thesis study not only includes MINLP and stochastic modeling approaches in microalgae-based biofuel and biomass production, but also provides a versatile and holistic modeling framework that can guide planning and decision-making processes in industrial-scale production. The fact that the developed models provide consistent results at different stages demonstrates their validity at the theoretical level; however, future experimental studies and field data are of great importance in order to evaluate the applicability of the models to real systems. With applied research to be conducted in this direction, the validation of the models and their integration into industrial systems will become possible. On the other hand, the integration of stochastic structures in the face of the variability and uncertainties inherent in large-scale production planning and bioprocess systems increases the flexibility of the models, and this situation is important in terms of sectoral applications.

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BIOGRAPHY

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