



UNIVERSIDAD
NACIONAL
DE COLOMBIA

Análisis del impacto económico de control predictivo basado en modelo económico en fotobiorreactores

Yulánderon Salguero Rodríguez
Ingeniero Químico

Universidad Nacional de Colombia
Facultad de Minas, Departamento de Energía Eléctrica y Automática
Medellín, Colombia
2018

Análisis del impacto económico de control predictivo basado en modelo económico en fotobiorreactores

Yulánderon Salguero Rodríguez
Ingeniero Químico

Tesis o trabajo de investigación presentado como requisito parcial para el título de:
Magister en Ingeniería – Automatización Industrial

Directores:

Ph.D. Jairo José Espinosa Oviedo

Ph.D. Cesar Augusto Gómez Pérez

Línea de investigación:

Modelamiento y control de sistemas dinámicos

Grupo de investigación:

Grupo de automática de la Universidad Nacional (GAUNAL)

Universidad Nacional de Colombia

Facultad de Minas, Departamento de Energía Eléctrica y Automática

Medellín, Colombia

2018



UNIVERSIDAD
NACIONAL
DE COLOMBIA

Analysis of the economic impact of economic model predictive control in photobioreactors

Yulánder Salguero Rodríguez
Chemical engineer

Universidad Nacional de Colombia
Facultad de Minas, Departamento de Energía Eléctrica y Automática
Medellin, Colombia
2018

Analysis of the economic impact of economic model predictive control in photobioreactors

Yulánderon Salguero Rodríguez
Chemical engineer

Thesis or research work presented as partial requirement for the title of:
Master of Engineering – Industrial Automation

Advisors:

Ph.D. Jairo José Espinosa Oviedo

Ph.D. Cesar Augusto Gomez Perez

Research line:

Modelling and control of dynamic systems

Group of research:

Grupo de automática de la Universidad Nacional (GAUNAL)

Universidad Nacional de Colombia

Facultad de Minas, Departamento de Energía Eléctrica y Automática

Medellin, Colombia

2018

“Biofuels, carbon capture, winds, fission, fusion it does not really matter but it has to be clean, cheap and scalable”

Bill Gates

Acknowledgments

Firstly, I would like to express my sincere gratitude to my advisors: Professor Ph. D Jairo Jose Espinosa Oviedo and Professor Ph. D. Cesar Augusto Gomez Perez of the Department of Electrical Energy and Automatic, Faculty of Mines at Universidad Nacional de Colombia, Medellin Campus for all their immense knowledge, continuous support, addressing and especially for their patient. The doors to their offices were always open whenever I ran into problems or I had question about this work or writing.

I would also like to thank to the researchers: Ph. D. Alejandro Marquez Ruiz and Ph. D. Richard Rios Patiño. They helped me a lot during this project with their knowledge regarding to: modelling, simulation and control of dynamical systems.

I thank to all the GAUNAL group, for the stimulating discussions, knowledge, kind support and for all the fun we have had in the last years. Especially to the Ph. D. students Andres Felipe Acosta Gil and Semaria Ruiz Alvarez, for helping me when I needed the most using Matlab and Simulink for simulation purposes, data processing among many other situations.

I am deeply grateful to the Administrative Department of Science, Technology and Innovation (COLCIENCIAS) and Universidad Nacional de Colombia for the financial support of this project through the following programs:

- Young researchers program 2014 in Colombia “Convocatoria Jóvenes Investigadores e Innovadores No. 645 de 2014”.
- Young researchers program 2015 in Colombia “Convocatoria Jóvenes Investigadores e Innovadores No. 706 de 2015”.
- Postgraduate scholarship “Mejores trabajos de grado en la Universidad Nacional de Colombia 2015”.
- Postgraduate Scholarship granted by the Faculty of Mines.

I want to thank also to *Universidade Estadual de Campinas* (UNICAMP) and “Red de Macrouniversidades de América Latina y el Caribe” for the financial support of this research project through “IX Convocatoria de Movilidad en el Posgrado”.

My sincere thanks also goes to Professor Ph. D. Luz Adriana Alvarez Toro of the *Departamento de Engenharia de Sistemas Químicos (DESQ), Faculdade de Engenharia Química (FEQ)* at *Universidade Estadual de Campinas* (UNICAMP), Campinas Campus in Brazil. She provided me an opportunity to join her team as intern, and who gave me access to her Research Group and Laboratories.

I would like to express my gratitude to the group of *Laboratório de Controle e Automação de Processos* (LCAP) at UNICAMP. Especially to the doctoral student Romero Florentino de Carvalho and the master students Flávio Augusto Rossi Violaro, Raissa Costa de Oliveira and Daniel Martins Silva for their support learning portuguese and Model Predictive Control.

I thank to all my friends at King Abdullah University of Science and Technology (KAUST) for the knowledge, discussions, kind support, suggestions and for all the fun we have had in the last year in Saudi Arabia. Especially to the Ph. D. student Rodrigo Jose Jimenez Sandoval, the Master student Abdulrahman Abdulrashid Hamed Hashim and the Mechatronics engineer Javier Fernando Garnica Molina.

I would also like to thank to my colleagues and friends: Chemical Engineer Carlos Alberto Rivera Corredor, and Ph. D. Sandra Milena Lopez Zamora for all the stimulating discussions, support and suggestions related with this research project.

Finally, but not least important, I must express my very profound gratitude to my family: my father Guillermo Salguero Nieto, my mother Patricia Rodriguez Gonzalez, my brother the petroleum engineer Eric Fernando Salguero Rodriguez, my sister the nurse Norida Salguero Rodriguez and my godmother Ana Elvia Salguero Nieto. They provided me with unfailing support, motivation and continuous encouragement throughout my master studies and through the process of writing this thesis. This accomplishment would not have been possible without them. Thank you.

Abstract

In this thesis it was proposed a formulation to evaluate the economic impact of the use of Economic Model Predictive Control (EMPC). For this, a model of a photobioreactor (PBR) was proposed by combining different phenomena within the reactor for the cultivation of microalgae such as: fluid dynamics, photosynthesis kinetics and mass balances. The proposed model has a new characteristic, it is the inclusion of an empirical equation which takes into account the performance of the Light - Dark cycles in a dynamic mathematical model for the predictions of productivity in the PBR. Besides of that, an economic optimization was proposed, which takes into account both the pumping energy of the system and the energy produced, by translating the productivity of biomass to energy, through some expressions proposed in this thesis, this expression combined with the model previously proposed is able to reach optimal regions for the PBR operation in accurate way. Finally, it was found that the economic impact of the use of economic control was positive for the system, due to the fact that its objective function and prediction model take into account not only the productivity of the system, but also the energy costs associated with pumping and mixing.

Key words: Photobioreactor, Photosynthesis, Light - Dark cycles, Microalgae, PSU model, EMPC.

Resumen

En esta tesis se propuso una formulación para evaluar el impacto económico del uso del control predictivo basado en modelo económico (CPBME). Para ello, se propuso un modelo para un fotobiorreactor (FBR) combinando diferentes fenómenos dentro del reactor para el cultivo de microalgas tales como: dinámica de fluidos, cinética de fotosíntesis y balances de materia. El modelo propuesto tiene una nueva característica, esta es la inclusión de una ecuación empírica la cual toma en cuenta el desempeño de los ciclos luz – oscuridad en un modelo matemático de carácter dinámico para las predicciones de la producción en el FBR. De igual forma, se propone una optimización económica, en la cual se tiene en cuenta tanto la energía de bombeo del sistema, como la energía producida, al traducir la productividad de la biomasa a energía, por medio de algunas expresiones propuestas en esta tesis. Al combinar la optimización y el modelo propuesto es posible establecer de forma precisa regiones de funcionamiento óptimo para el sistema de FBR. Finalmente, se encontró que el impacto económico del uso de control económico fue positivo para el sistema, ya que a través de su función objetivo y modelo de predicción se tenía en cuenta no sólo la productividad del sistema, sino también los costos energéticos asociados con el bombeo, agitación y mezclado.

Palabras clave: Fotosíntesis, ciclos luz-oscuridad, microalgas, modelo PSU, CPBME.

Content

	Pag.
Abstract.....	XI
List of figures.....	XV
List of tables	XVIII
Introduction	1
1. Chapter 1: State of the art.....	3
1.1 Microalgae Cultures.....	3
1.1.1 Classification of cultures according to mode of operation.....	4
1.1.1.1 Open reactors	4
1.1.1.2 Closed reactors.....	5
1.1.2 Operation of PBR and economic problems.....	7
1.2 Advances in process control	9
1.2.1 Model predictive control (MPC)	11
1.2.2 Economic Model Predictive Control - EMPC	12
2. Chapter 2: Agitation and mixing design.....	15
2.1 Illumination in PBR design and modelling	15
2.2 Agitation and mixing in PBR.....	17
2.3 Mixer proposed and CFD simulation	18
2.3.1 Turbulence model	19
2.3.2 Swirl number.....	20
2.3.3 Static mixer proposed.....	21
3. Chapter 3: Dynamic model of the photobioreactor.....	31
3.1 Modelling of the photobioreactor.....	31
3.1.1 Description of the Photobioreactor	32
3.1.2 Dynamic model of the photobioreactor	34
3.1.3 Kinetics of photosynthesis.....	37
3.1.4 Illumination and light – dark cycles model.	40
3.2 Results of dynamic model with LD cycles and PBR	50
3.2.1 Disturbance of external illumination.....	53
3.2.2 Disturbance of biomass concentration in the input of PBR	56
3.2.3 Disturbance of velocity	58
3.2.4 Comparison of some variables of the PBR model with the literature....	61
4. Chapter 4: Photobioreactor control strategies.....	63

4.1	Model predictive control and economic model predictive control in photobioreactors	64
4.1.1	Model predictive control - MPC	64
4.1.2	Energetic function	67
4.1.3	Economic Model predictive control - EMPC	68
4.2	Results of the MPC and EMPC controllers	71
4.2.1	Reference Tracking MPC.....	71
4.2.2	Scenario 1	73
4.2.3	Scenario 2	77
4.2.4	Comparison of MPC and EMPC performance.....	81
4.2.5	EMPC with Colombian currency in first scenario.....	84
5.	Chapter 5: Conclusions and future work	89
5.1	Conclusions.....	89
5.2	Products of this thesis	90
5.3	Future work	90
6.	References	91
A.	Annex A: Pressure drop	99
B.	Annex B: Numerical details and comparison of control strategies.....	102

List of figures

	Pág.
Figure 1-1: Microalgae culture in open reactors.....	4
Figure 1-2: Tubular PBR.....	5
Figure 1-3: Bubble column PBR.	6
Figure 1-4: Flat panel PBR.	6
Figure 2-1: Diagram of the reactor for the simulation.	18
Figure 2-2: Cross-sectional area of the PBR.	21
Figure 2-3: Static mixer proposed for the PBR.....	21
Figure 2-4: Geometry of the PBR without mixers.....	22
Figure 2-5: Profiles for the reactor without mixer a) velocity z-y view b) velocity x-y view c) velocity z-x view d) pressure drop.....	23
Figure 2-6: Study geometry used in COMSOL with static mixer.	24
Figure 2-7: Profiles for the reactor with one static mixer a) velocity z-y view b) velocity x-y view c) velocity z-x view d) pressure drop.....	25
Figure 2-8: Swirl number profile as a function of length for various linear velocities using one static mixer a) 0.1 m/s b) 0.15 m/s c) 0.2 m/s d) 0.25 m/s e) 0.3 m/s f) 0.35 m/s g) 0.4 m/s h) 0.45 m/s i) 0.5 m/s.	26
Figure 2-9: Velocity profile with different spacing a) 50 cm b) 80cm	27
Figure 2-10: Profile swirl number with different spacing a) 50 cm b) 80cm.	28
Figure 2-11: Geometry of the reactor with four mixers.	28
Figure 2-12: Profiles for the reactor with four static mixers a) velocity z-y view b) velocity x-y view c) velocity z-x view d) pressure drop.....	29
Figure 2-13: Swirl number profile for some static mixers.	30
Figure 3-1: Diagram of the PBR.....	32
Figure 3-2: Diagram of the solar receiver.....	33
Figure 3-3: Diagram of the solar receiver divided into sections.....	34
Figure 3-4: Schematic representation of kinetic models based on PSU.....	38
Figure 3-5: Cross-sectional area of the PBR	41
Figure 3-6: Trajectory on the vertical axis for a) $v = 0.55$ m/s b) $v = 0.1$ m/s	42
Figure 3-7: Illumination profile in the cross-sectional area PBR.....	42
Figure 3-8: Illumination received by the microalgae. For a) $v=0.55$ m/s b) $v=0.1$ m/s.....	43
Figure 3-9: Signal of illumination in the frequency domain a) $v = 0.55$ m/s extended (0.01 Hz - 2.0 Hz). b) $v = 0.1$ m/s extended (0.01 Hz - 2.0 Hz).	44
Figure 3-10: System frequencies a) first frequency b) second frequency c) third frequency.	45

Figure 3-11: Power spectrum of the frequencies a) first frequency b) second frequency c) third frequency.	46
Figure 3-12: Attenuation as function of biomass concentration	47
Figure 3-13: Attenuation as function of biomass concentration prediction model.....	48
Figure 3-14: Attenuation for different external illumination and biomass concentration...	49
Figure 3-15: Illumination as function of time.	50
Figure 3-16: LD cycles simulation, illumination profile a) zoom 20000s – 21600 s b) zoom 21000s – 21600 s.	51
Figure 3-17: Carbon dioxide concentration output of the PBR.....	52
Figure 3-18: Product Dynamics a) Biomass concentration b) oxygen concentration	52
Figure 3-19: Disturbance on external illumination.....	53
Figure 3-20: LD cycles prediction a) 0s – 32400 s b) zoom 10000s – 32400 s.....	54
Figure 3-21: Biomass concentration output of the reactor a) 0s – 32400 s b) zoom 10000s – 32400 s	54
Figure 3-22: Oxygen concentration output of the reactor a) 0s – 32400 s b) zoom 10000s – 32400 s.....	55
Figure 3-23: Carbon dioxide concentration output of the reactor a) 0s – 32400 s b) zoom 10000s – 32400 s	55
Figure 3-24: Initial biomass concentration disturbance.....	56
Figure 3-25: LD cycles prediction, illumination inside the culture a) 0s – 32400 s b) zoom 10000s – 32400 s	56
Figure 3-26: Biomass concentration in the output of the PBR 0s – 32400 s.	57
Figure 3-27: Oxygen concentration in the output of the PBR a) 0s – 32400 s b) zoom 10000s – 32400 s	57
Figure 3-28: Oxygen concentration in the output of the PBR a) 0s – 32400 s b) zoom 10000s – 32400 s	58
Figure 3-29: Disturbance of velocity for the system.....	58
Figure 3-30: Illumination profile and LD cycles a) 0s – 32400 s b) zoom 10000s – 32400 s.....	59
Figure 3-31: Biomass concentration in the output of the PBR a) 0s – 32400 s b) zoom 10000s – 32400 s	59
Figure 3-32: Oxygen concentration in the output of the PBR a) 0s – 32400 s b) zoom 10000s – 32400 s	60
Figure 3-33: Carbon dioxide concentration in the output of the PBR a) 0s – 32400 s b) zoom 10000s – 32400 s.....	60
Figure 4-1: Control scheme MPC.....	64
Figure 4-2: Control scheme EMPC.....	69
Figure 4-3: MPC reference tracking Ref = 0.005 mol/l a) Oxygen concentration b) Biomass concentration c) Velocity.....	72
Figure 4-4: MPC reference tracking Ref = 0.0055 mol/l a) Oxygen concentration b) Biomass concentration c) Velocity.....	73
Figure 4-5: Day operation profile a) Illumination b) biomass concentration.....	74

Figure 4-6: MPC results for scenario 1 a) Oxygen concentration b) Biomass concentration c) Velocity	75
Figure 4-7: EMPC results for scenario 1 a) biomass concentration b) velocity.....	76
Figure 4-8: Comparison of results for scenario 1 a) biomass concentration b) velocity ..	76
Figure 4-9: Scenario 2, variation of initial biomass a) disturbance b) biomass concentration.....	78
Figure 4-10: MPC results for scenario 2 a) Oxygen concentration b) Biomass concentration c) Velocity	79
Figure 4-11: EMPC results for scenario 2 a) biomass concentration b) velocity.....	80
Figure 4-12: Comparison of results for scenario 1 a) biomass concentration b) velocity	81
Figure 4-13: Results for first scenario EMPC with COP a) biomass concentration b) velocity	85
Figure 4-14: Comparison of results for first scenario: Open loop, EMPC, MPC and EMPC - COP a) biomass concentration b) velocity	86
Figure 6-1: Pressure drop as function of velocity	99
Figure 6-2: Pressure drop as function of square of velocity	101

List of tables

	Pág.
Table 2-1: Model parameters turbulence model.....	20
Table 3-1: Parameters of the kinetic model.....	39
Table 3-2: Parameters of the attenuation model.	41
Table 3-3: Parameters of the identified function for attenuation.	48
Table 3-4: Parameters for PBR simulation.....	51
Table 3-5: Comparison of frequencies of LD cycles.....	62
Table 3-6: Comparison of specific growth rate of PBR.....	62
Table 4-1: Summary first scenario control strategies applied to PBR.....	82
Table 4-2: Summary second scenario control strategies applied to PBR.....	83
Table 4-3: Summary first scenario in COP: Open loop, EMPC, MPC and EMPC – COP.....	87
Table 4-4: Variations first scenario: EMPC, MPC and EMPC – COP.....	87
Table 6-1: Summary first scenario in COP: Open loop, EMPC, MPC and EMPC – COP.	103

Introduction

During the last two decades, photobioreactors (PBRs) have presented significant advances regarding to modeling, design and control. It was motivated by the global context and the change of paradigms in sources for energy supply, those systems have achieved reductions in energy consumption and resources. Nevertheless, those systems still operate inefficiently, due to high operational costs that make them unfeasible in an industrial scale.

The main problem with industrial PBRs lies in the high operational costs, which make them unfeasible at industrial levels. According to some authors, control strategies can be an adequate strategy in order to improve economy of PBR. Some applications of process control over PBR have been presented, ranging from classical regulatory control (PID), to the use of sliding mode control, and the use of model predictive control (MPC).

Recently, the use of control strategies on these systems has been studied, applying Model Predictive Control for the management of multiple variables. Even, the application of Economic Model Predictive Control (EMPC) has been addressed, achieving improvements in the performance of PBR. However, the economic impact achieved by these advanced control strategies is currently unknown. Taking into account that the EMPC is a system that may have additional expenses for its application in PBR and that PBR require a considerable improvement to reach their economic feasibility. It is thus necessary to analyze if it is worth taking these systems to an economic control strategy, or if on the contrary the application of an EMPC does not produce any worth improvement that indicates that the use of a classic regulatory control is enough to obtain results close to the economic optimum of the system.

In the last two years, advanced control strategies such as EMPC have been studied, without studying the benefit of their use over classical control. In addition, it is important to note that, in the EMPC area, there are few reports in the microalgae culture area, mainly because it is an idea that has been under development for a short time. As a result, PBRs are an adequate system to evaluate the economic impact that can be achieved with EMPC.

Additionally, although there are some recent reports related to the application of these control strategies, the study of their impact on the economy of the process is unknown, or has been addressed in a superficial way. The application of economically feasible PBRs in the bioprocess industry will depend on the small details in which can be saved resources, in this sense control systems can reduce energy consumption or improve the performance of the system.

Objectives of this thesis:

1- General objective:

To analyze the economic impact of the implementation of a control scheme with Economic Model Predictive Control (EMPC) applied to photobioreactors.

This thesis is developed as follows:

- Chapter 1: it is presented the state of the art in order to show the research effort in the field of microalgae, photobioreactors and control applied to microalgae culture. Also it is highlighted the current open research problems.
- Chapter 2: this chapter presents a static mixer design, which was developed specially for reducing energy consumption in the photobioreactor and improving the productivity.
- Chapter 3: it is shown a proposed dynamic photobioreactor model which takes into account the effect of Light-Dark cycles on the productivity. Also, it was included the agitation and mixing effect achieved by the static mixer proposed previously.
- Chapter 4: it is presented the control strategies in order to improve the economic performance of the photobioreactor. Also it is presented a proposed function and variables used for evaluating an energetic function of the system.

Chapter 1: State of the art

This chapter introduces the main research efforts and some concepts for understanding the developed research, it is presented as follows:

- Firstly it is explained generalities about of microalgae cultures, open systems, closed systems and economic challenges for photobioreactor (PBR) operation.
- Secondly, it is shown generalities regarding to process control applied to microalgae cultures.

1.1 Microalgae Cultures

Microalgae are a diverse group of prokaryotic and eukaryotic photosynthetic organisms, with a simple structure, which allows them a quick growth (Bitog et al., 2011) and to produce diverse organic compounds. For their growth they need carbon dioxide, light source and sources of nitrogen, phosphorus and other nutrients, these raw materials are very cheap, as light and CO₂ are found in nature, sources of nitrogen and phosphorus can come from different waste sources. This makes the cultivation of microalgae an interesting process for the present and future, moreover, this process is friendly with the environment and offer us the possibility of fixing atmospheric CO₂, which causes the greenhouse effect and global warming. Diverse products can be obtained from microalgae cultures, such as: essential oils (used in the food industry), cosmetics, pharmaceuticals and biofuels. Unfortunately, the cultivation of microalgae still presents some technological problems that affect the performance of the process. As a result, when microalgae culture is scaled up, productivity decrease and operation cost increase in a dramatic way (Lehr & Posten, 2009).

The cultivation of microalgae is not a new practice. Its study goes back to the time of the Second World War (Bitog et al., 2011), in which it was proposed as a protein supplement, later, the research was redirected towards the possibility of obtain biofuels from these

organisms, this fact led to several studies on the culture in order to obtain several types of fuels.

Currently, microalgae can play an important role in the concept of biorefineries (González-Delgado & Kafarov, 2011), due to it, they can be used as raw material to obtain a wide variety of products such as: biodiesel, ethanol, hydrogen, protein for the concentrate of animals (Posten & Schaub, 2009), omega 3 and omega 6 oils and special products like chlorophyll, beta-carotenes and C-phycoocyanin (Harun, Singh, Forde, & Danquah, 2010).

1.1.1 Classification of cultures according to mode of operation

The industrial scale production of microalgae can be carried out through two types of operation, those are open reactors and closed reactors or PBRs (Brennan & Owende, 2010).

1.1.1.1 Open reactors

Cultivation in open reactors is the most frequently used practice for the production of biomass from microalgae. Among these reactors are some originated naturally such as: lagoons, wells, lakes. One of the most widely used open bioreactors is the runway pond (see figure 1-1), where the fluid with and microalgae go through the pond with a depth of 0.2 m - 0.5 m (Brennan & Owende, 2010). These track ponds have closed circuits with oval shape and recirculation channels. They allow a continuous mixing that stabilizes the growth of the microalgae and therefore their productivity, for this reason, the pond has impellers of flow with the form of pallets and a continuous feeding of air, to provide the CO₂ for the culture.

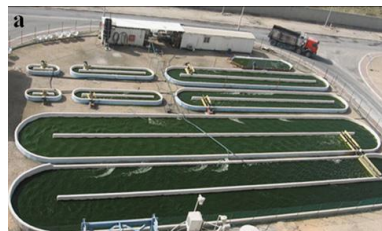


Figure 1-1: Microalgae culture in open reactors.

Taken from Bitog et al (Bitog et al., 2011).

In comparison to closed systems, open systems are cheaper and simpler technology to implement for large-scale production, they require less energy and their maintenance is easy to perform (Brennan & Owende, 2010). However, this type of systems have certain operating problems, due to extensive areas used and their exposure to the environment, which can cause contamination of the culture, affecting in a negative way products that have cosmetic and food purposes, generating bad odors and affecting productivity (Singh & Sharma, 2012; Suh & Lee, 2003). The productivities achieved in open cultures are low, due to the difficulty of controlling optimal conditions in the culture medium, which can present drastic variations with negative effects on microalgae growth.

1.1.1.2 Closed reactors

PBRs are devices that differ from open systems, in the fact that they try to increase the area of light incidence, to benefit the contact of microalgae with photons, it means, to achieve a high surface to volume ratio (Suh & Lee, 2003). Its main advantage over open systems is the possibility of controlling the process variables and obtaining better productivity (Brennan & Owende, 2010). There is a great variety of designs in the literature, Posten (2009) states that there are three large families of PBR: tubular reactors, bubble columns and flat screen reactors.

Tubular reactors are tubes with considerable extension, located parallel, allowing the efficient incidence of light, as shown in Figure 1-2. The use of tubes favors a high surface-volume ratio, which is one of its main advantages (Posten, 2009). The scale up of those reactors is simple. However, the necessary extension for the process generates important gradients and consequently important changes in the process variables (Molina, Fernández, Ación, & Chisti, 2001). It is relatively inexpensive, as the materials for its construction do not need to be very specific, but the cleaning of the reactor can be very complex.



Figure 1-2: Tubular PBR.

Taken from Bitog et al. (Bitog et al., 2011).

Bubble column PBR are devices with form of columns where the culture is located, and the gas that provides the CO_2 is continuously fed, its main advantage is the optimization of the mass transfer, through the aeration system (X. Wu & Merchuk, 2002). This type of reactors do not have a high surface-volume ratio. In Figure 1-3 those columns are shown.



Figure 1-3: Bubble column PBR.

Taken from Bitog et al (Bitog et al., 2011).

Flat panel PBR are intermediate systems, which combine the flow capacity of the tubular reactor, and the aeration efficiency of the bubble columns. As well as, a maximization of the incident light area (Su, Kang, Shi, Cong, & Cai, 2010). In Figure 1- 4, the flat panel device is shown.

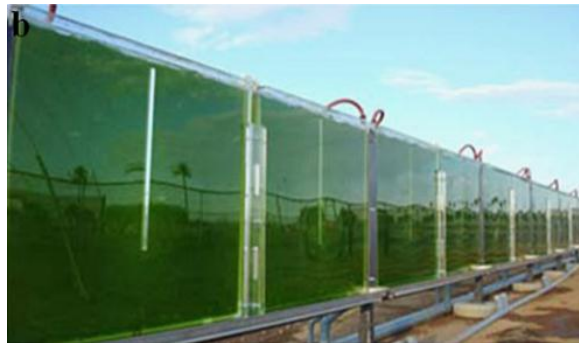


Figure 1-4: Flat panel PBR.

Taken from Bitog et al (Bitog et al., 2011).

In the literature, the progress in terms of simulation for the three types of reactors has been reported, in some cases with their respective validation. However, tubular PBR have already been carried out on a pilot scale and their simulation performance has been contrasted with the real performance of the system (Fernández et al., 2014), showing good

performance and results consistent with the simulations. This is why, this thesis is focused on tubular PBR as suitable equipment for modeling, simulation and control purposes.

1.1.2 Operation of PBR and economic problems.

PBR application in biorefineries and bioprocess industries need lots of engineering efforts in order to solve many issues. For instance, some authors like Posten and Lehr (Lehr & Posten, 2009) mention that operation cost should be reduced substantially in order to improve economy of the process. The operation and design of PBR must improve taking into account all variables related to the economy of the process. This is a hard task, because the PBR presents the interaction of different phenomena such as: illumination, refraction, mass transfer, fluid dynamics and photosynthesis. Better mathematical models can be used in order to design, control and optimization purposes. Several modern tools have been used for the PBR analysis such as: CFD (Gómez-pérez, Espinosa, Ruiz, & Boxtel, 2015), modern control design (Fernández et al., 2016) and optimization methods (Soman & Shastri, 2015). Currently there are some pilot PBR functional. However, for the scale-up of those PBR still remains dramatic reductions of productivity, there is not an economically feasible PBR for large scale at this moment (Chen, Xu, & Vaidyanathan, 2018).

In the PBR field, still there are some challenges to solve. Some researchers have evaluated the PBR process using economic aspects (Lehr & Posten, 2009; Posten, 2009). It was found that the productivity reached in the PBR is not enough taking into account the energy requirements of the operation process, such as: pumping, mixing and aeration. Sensitivity analyses showed (Norsker, Barbosa, Vermuë, & Wijffels, 2011) that mixing takes most of the energy required by the PBR in its operation, and due to it, mixing has a huge effect in the economy of this process. Usually, other reactors do not show high agitation and mixing costs, but taking into account that raw materials for microalgae cultivation such as: carbon dioxide and illumination can be taken from the environment, those cost became really significant.

The biorefineries are a new concept under many research and challenges; there are biorefineries with terrestrial crops to obtain liquid fuels, such as: bioethanol and biodiesel, nevertheless, those competes for water and energy (Giwa et al., 2018). It is thus necessary to develop biorefineries which do not be an environmental burden in terms of feedstocks

and postprocessing of materials. For future scenarios of microalgae culture it is required a sustainable operation, achieving a production energetically sustainable for PBR, which can led to new biorefineries. Due to the above, there are lot of effort to improve PBR operation in order to obtain an economically feasible operation of those systems.

PBRs are devices that allow better control over the important variables in the growth of microalgae cultures, in comparison to open systems. In spite of the above, the cultivation of microalgae is a practice that is still economically unfeasible, due to the facts that: the construction of PBRs is very expensive, the actual productivities obtained in those systems are low, the costs of operation, separation and extraction can reach high values, and for all of those reasons the profitability does not compensate the operating costs (Cesário, da Fonseca, Marques, & de Almeida, 2018; Lehr & Posten, 2009).

In the chemical and biological processes, a very changing panorama has been presented regarding the prices of raw materials, energy sources, product specifications and markets. Additionally, those process industries are constantly developing and becoming more competitive, this fact makes it more difficult to grow and to remain in the global market. (Medianu & Popescu, 2012). Because of that, industry requires in future scenarios more efficient and sustainable process.

In his review presented in 2009 (Posten, 2009), Posten analyzes some factors that can be considered in the improvement of the economy for microalgae culture in PBRs. In the first place, he mentions the analogy with traditional agriculture, emphasizing that nature is capable of handling all the difficulties that are present in PBRs, such as: fluid transport, mass transfer, light incidence and even processes of separation; and so he proposes to continue studying the phenomena present in nature to improve the system. As a second option, Posten also highlights the increase of the surface exposed to lighting, this taking into account its high influence on the performance of those systems. Another option proposed by him is the improvement in the process of agitation and air supply, which leads to high costs currently and losses in the process. Finally, Posten mentions that the use of modeling and control tools in PBRs can improve the design and operation of those systems.

PBR performance has been optimized through experimental work. Besides of that, other engineering tools for optimization has shown interesting results like the use of CFD for

agitation and energy consumption analysis (Gómez-pérez et al., 2015) reducing pumping energy and flows for its operation. On the other hand, some advanced control strategies such as Model Predictive Control (MPC) has been becoming an important tool, a correct design of MPC can reduce raw materials for the process and energy consumption (Fernández et al., 2016).

All the factors mentioned in this section make the PBR industrial operation economically unfeasible. According to the possibilities of improvement of these systems exposed in 2009 (Posten, 2009), process control applied to PBRs is a strategy that achieves significant improvements, whereby we focus on the applicability of control to address the problem of economic feasibility. This problem has been described for more than ten years, even so, it still remains as an open research problem in this field.

1.2 Advances in process control

In the chemical processes, a very changing panorama has been presented regarding the prices of raw materials, energy sources, product specifications and markets. Additionally, the chemical process industries are constantly developing and becoming more competitive. This fact makes it more difficult to grow and to remain in the global market. Therefore, the control and optimal operation in chemical processes in the industry has received special attention in the last two decades (Medianu & Popescu, 2012).

The importance of a control that allows the supervision of an industrial process is manifested when an operator is hardly able to deduce the optimal operating conditions, due to the number of variables and the high complexity of the process. The most common practice at industrial level is to control a unit, mainly because it is an easy strategy to understand for the operators and engineers in charge (Minasidis & Johannes, 2013).

In the past, the main objective of control was the stability of chemical process systems. However, currently control strategies are focused on efficiency and productivity (Medianu & Popescu, 2012). The requirements and quality of the products must be improved in the chemical industries, the optimal control strategies must be implemented, because they are the real option to operate a chemical process with an optimal productivity, minimizing the consumption of resources and energy costs (Marquez, Gomez, Deossa, & Espinosa, 2011).

The search for a trusted control system for the safe and economic operation of chemical processes has been one of the main worries in the field of engineering and research. Currently, the function of control systems in chemical processes makes more than the basic processes of monitoring and regulation, even operating the process in a range, maintaining the quality of products and optimizing production (García, Fernandez-Anaya, Vargas-Villamil, & Orduña, 2010).

In the literature there have been few reports related to the application of control in PBRs, and those have come in a gradual increase during the last decade. It is important to highlight that the PBRs have been in a growing development the last two decades, so there are still problems of study in this system, and therefore process control is increasingly linked to it.

In the chemical processes, there are usually multiple phenomena such as: mass, energy and momentum transfer, which are strongly coupled. This causes the existence of multiple variables in those systems, with ranges for their values, due to operational restrictions, or the principles that govern these phenomena. All this led to the research towards model-based predictive control (MPC), which is an adequate strategy to take into account multiple inputs, outputs and restrictions (Amrit, 2011). Specifically in the case of PBRs, it is presented the flow of fluids, mass transfer and the reaction phenomena taking advantage of the illumination of the culture medium, which brings a complexity that can be approached with this type of control (Becerra-Celis, Hafidi, Tebbani, Dumur, & Isambert, 2008).

During the first decade of the XXI century, the first advances in process control applied to PBRs were presented. Those searching improvements of the economic conditions for the process operation. Among those, we can mention some control systems whose objective was to maintain the density at a desired level by manipulating the inflow and concentrations. In that sense the application of PID was initially reported, and subsequently, MPC for those systems (Becerra-Celis et al., 2008). It allows to properly manage those systems taking into account the previously mentioned considerations and reducing operating costs, and the CO₂ losses from the system.

In the second decade of the current century, applications of other types of controllers to this chemical process system were presented, such as: the use of sliding modes control (Andrade, Pagano, Fernández, Guzmán, & Berenguel, 2014), control by passivity (Uyar &

Kapucu, 2015), and a variant of the MPC to treat the system non-linearly (Benattia, Tebbani, Dumur, & Selis, 2014). Most of those in order to control the concentration of biomass by manipulating the dilution rate in the system, which allows to improve the productivity achieved by the system.

There is a current effort of research in order to improve PBR performance. According to previous studies, control strategies application to those systems can help to solve this problem. Due to it, we focus on the application of modern control strategies such as: model predictive control (MPC) and economic model predictive control (EMPC) on PBR. Those control strategies are used when the process is complex, it presents constraints for its variables and there are multiple variables, this is the case of the microalgae culture.

1.2.1 Model predictive control (MPC)

The concept of Model Predictive Control - MPC has a long history. In 1970 Shell Oil engineers developed their own MPC technology, with an initial application in 1973 (Richalet, Rault, Testud, & Papon, 1978). In one of the review presented in 2010, Holkar et al. (Holkar & Waghmare, 2010) mention that in 1989 a document was published that addressed different MPC techniques. This highlighted the advantages in design and implementation in relation to quadratic linear control. The application of MPC to non-linear systems was also shown. Subsequently, in 1999 a robustness report was published in MPC, and techniques for the management of restrictions, stability and performance were proposed.

Some advances in the last two decades are also mentioned in the Holkar et al. review report (Holkar & Waghmare, 2010), among those: it is mentioned that Sandoz et al (Sandoz, Desforges, Lennox, & Goulding, 2000) presented a paper at the beginning of the XXI century with various methods to be used with MPC schemes, such as: quadratic programming and long-range quadratic programming. Also, in 2003, Kimiaghalam et al (Kimiaghalam, Ahmadzadeh, Homaifar, Sayarrodsari, & Technologies, 2003) proposed a suitable formulation for indirect adaptive control algorithms, it was presented with real-time application of MPC to improve the properties at computational level.

In the years 2006 and 2007 some articles were also presented in which it was reviewed the robust MPC with methods based on model uncertainties. Comparisons have also been made of some MPC techniques (Mayne, 2014). The advance in the field of MPC has been

considerable during the last decades, and more information regarding its development can be found in some published review documents related to advances in this field (Michael G. Forbes, Patwardhan, Hamadah, & Gopaluni, 2015; Holkar & Waghmare, 2010; Mayne, 2014).

The main advantages of MPC over PID controllers are their ability to handle restrictions, non-minimum phase processes, changes in system parameters (robust control) and their direct applicability to multivariable processes (Mayne, 2014). The MPC, rather than a control technique in itself, is a control methodology with the following characteristics (M. G. Forbes, Patwardhan, & Gopaluni, 2015):

- a) Explicit use of a model to predict the output of the process in future moments of time (horizon).
- b) Management of restrictions for both input and output variables.
- c) Calculation of the control signals by minimizing a certain objective function.
- d) Sliding strategy, so, at each moment the horizon moves towards the future. Which implies applying the first control signal at each moment and discard all the rest, repeating the calculation at each sampling time.

The MPC has shown good results in its applicability in processes for the regulation of variables, however it does not ensure the operation of the system in optimal points on economic terms. This has been one of the main concerns that promoted the idea of an MPC control that directly included economic considerations, which gave way to Economic Model Predictive Control - EMPC.

1.2.2 Economic Model Predictive Control - EMPC

In process control, a two-layer architecture has been studied to consider the economic optimization of a system (Marquez, Patiño, & Espinosa, 2014). Usually, this structure is composed of two layers. The first layer is responsible for the optimization of the reference points of the process, using models in steady state and economic considerations. The second layer is in charge of the regulatory control, which receives as a reference the values estimated in the upper level of optimization. In many of these systems the MPC is used (Marquez et al., 2014).

Despite the traditional approach, there are a significant number of systems and processes in which hierarchical discrimination separated from economic considerations and operational control objectives are ineffective, or not entirely correct. Due to the above, some strategies have been presented in order to overcome this situation. A complete review of this topic is presented by Ellis and colleagues (Ellis, Durand, & Christofides, 2014) and Tran et al. (Tran, Ling, & Maciejowski, 2014). One of those strategies is the called Economic Model Predictive Control (EMPC), a name proposed in the first measure for control applications in the management of power systems (Marquez et al., 2014). The main feature of the EMPC is the use of the economic cost function of the optimization layer directly as a cost function.

Several papers have been presented in the applications and properties of the EMPC, despite its relative novelty in the field of MPC. Among those studies can be found some related to energy management in smart grids, air conditioning systems and energy for constructions. Some applications in the design of sustainable policies have also been shown, addressing the problem of the impacts of climate change (Marquez et al., 2014). A distributed approach of EMPC for a network of nonlinear chemical processes has been reported (Santander, Elkamel, & Budman, 2016). In some documents, the development of EMPC strategies based on Lyapunov (LEMPC) is addressed for a certain type of non-linear systems (Heidarinejad, Liu, & Christofides, 2011).

Although the advances in EMPC cannot be unknown, some important questions still remain as open research problems. While some criteria have been addressed to guarantee the asymptotic stability of the EMPC, some situations such as the selection of the best design of the control system with economic objective without neglecting closed-loop convergence, stability or quantification of closed-loop performance. Those still are research problems that require more effort (M. G. Forbes et al., 2015; Marquez et al., 2014).

The performance of most of the different EMPC formulations in the literature is not completely known (Ellis et al., 2014; Tran et al., 2014). Also, due to the dynamic nature of the EMPC, there is a need of research in the assessment of disturbances and detection processes, isolation and the appropriate control structures to solve different types of failures. The operation of the MPC with restrictions is a subject that has been widely studied, however in the EMPC there are still some research problems open to exploration (Lee, 2014).

One of the motivations for the EMPC as an alternative to traditional hierarchical control is that it assumes that the system can reach an optimal stationary state, which is not entirely true, ignoring the transient state. Additionally, due to continuous dynamic perturbations, the process can never reach this state, invalidating one of the basic assumptions used in traditional calculations. The study of performance is a current challenge, since in EMPC a non-convex cost function is usually available, which may imply the existence of multiple minimums (Santander et al., 2016).

It is important to highlight that the additional benefit in economic terms, which can be achieved by the EMPC in a particular process, as in the case of PBRs, is not yet clear. The implementation of a very specific control scheme that requires modern knowledge can result in high costs in the process. In that sense, it is thus necessary to evaluate the economy of a particular process to define if the application of this control strategy can be significant or not.

During the last 3 years, other control strategies have been used in PBR, such as: economic hierarchical control (Fernández et al., 2015), control with robust MPC (Benattia, Tebbani, & Dumur, 2015), and MPC applied to PBRs (Pawłowski, Guzmán, Berenguel, Acien, & Dormido, 2018), in most of them a regulatory control strategies are combined and PID with optimizations, achieving an improvement in the performance of those systems. However, the analysis of the economic impact achieved by those control strategies is poorly discussed.

As it was presented in this chapter, PBR currently present high operational costs and many researchers have addressed this problem from different points of view, such as: optimization, modelling, control strategies, integrated designs and the combination of them. Agitation and mixing take values close to 70% of the energy consumption for this system, due to it, the next section presents an integrated design of a static mixer which improve hydrodynamic conditions inside the PBR and at the same time reduce energy consumption. It is a novelty of this work, in order to improve overall energy consumption.

Chapter 2: Agitation and mixing design.

This chapter proposed a new static mixer in order to improve hydrodynamic conditions for microalgae culture and reduce energy consumption. This section is organized as follows:

- Firstly, it is shown some research works related to the illumination in order to design PBR, as well as light-dark cycles importance.
- Secondly, it is presented an example of a static mixer of the literature, and its high pressure drop and energetic consumption.
- Finally, it is presented a new static mixer, which improves microalgae productivity without huge energy consumption.

2.1 Illumination in PBR design and modelling

Illumination is one of the most important factors that influence the growth of microalgae. For high levels in the concentration of biomass, the PBRs present internal light gradients, causing the cells to experience different light intensities depending on their location in the system between illuminated and dark areas. One consequence of light gradients in those systems is that algae are exposed to short light cycles when they move from light to dark areas (Hartmann, Béchet, & Bernard, 2014). The frequency of those cycles, known as Light-Dark (LD) cycles, is an important parameter of the illumination regime and it has an important influence on the efficiency of the use of light (Cheng, Huang, & Chen, 2014).

The concept of average illumination intensity allows us to find a variable for the PBR which depends on PBR configuration and cell concentration. So, the spatial configuration of the illumination regime inside the PBR is not important, because it is analyzed the average illumination intensity, a single value. Illumination can be estimated through a simple beer-lambert equation as follows:

$$I = I_0 e^{-\alpha \rho z}$$

Where I_0 is the external illumination on the surface of the culture ($\frac{\mu E}{m^2 s}$), α is the attenuation parameter ($\frac{m^4}{kg}$), ρ is the density of the fluid ($\frac{kg}{m^3}$), and z is the deep of the fluid inside the PBR (m).

The aim is to integrate the intensity of illumination into space and perform a weighting (Molina Grima, García Camacho, Pérez Sánchez, Ación Fernández, & Fernández Sevilla, 1997). An example is presented in the following expression:

$$I_{av} = \frac{1}{L} \int_0^L I(z) dz = \frac{I_0}{L} \int_0^L e^{-\alpha \rho z} dz = \frac{I_0}{\alpha \rho L} (1 - e^{-\alpha \rho L})$$

The average illumination intensity can be then used as a design parameter to be taken into account in the design of PBRs, because it identifies the state of the illumination regime for a given configuration. Molina et al. presented the concept and they evaluated the photosynthetic activity of the microalga *Isochrysis galvana* (Molina Grima et al., 1997). The average illumination intensity allows to perform the evaluation in a simple way, in another publication of Molina and colleagues (Molina Grima, Ación Fernández, García Camacho, & Chisti, 1999) the concept of total illumination analyzing a tubular PBR, it was characterized by two functions: one for the intensity of direct light and another for the intensity of diffuse light coming from the reflection of direct light. The volumetric integration of the functions over the volume of the PBR allows to find the average value.

On the other hand, other authors have worked the cycles of exposure to illumination, for example Park and Lee made their study of the effect of light pulsations in the species *Chlorella kessleri* (Park & Lee, 2000), the frequency of pulsations was investigated in comparison with a culture under continuous illumination condition. It was found that for frequencies lower than 1 kHz, the culture has a lower growth rate, with frequencies of 37 kHz, the culture has a higher productivity, and that it can have a greater effect on high density cultures, like those at industrial levels.

The high concentrations of biomass at industrial level generate illuminated and dark areas, which therefore generate LD cycles in the PBR, it depends of the configuration and hydrodynamics. In the work of Janssen et al. (Janssen, Tramper, Mur, & Wijffels, 2003), they studied the illumination regime and photosynthetic efficiency for different PBRs

identifying the areas where there are illuminated and dark areas. The hydrodynamics conditions inside the PBR depend of the configuration, size and agitation of the system, so the microalgae pass through the light and dark zones depending of the velocity profile that is generated inside the PBRs.

Mixing has shown to have a great influence on the growth in microalgae (Marshall & Huang, 2010), due to this, it is currently taken into account as a relevant factor for PBRs designs. An adequate mixing in this process prevents sediment formation, increases mass transfer, improves exchange between coexisting phases and improve the LD cycles conditions (Cheng et al., 2014).

The use of static mixers or flow obstacles with LD cycles has been studied in recent years. Mixers are an effective method that increases the degree of mixing inside the microalgae culture (Huang et al., 2015), allowing microalgae to move between illuminated and dark areas inside the reactor. LD cycle conditions enhance productivity in the system and cause a reduction in the photoinhibition. The productivity in biomass for PBRs using different static mixers increase between 30% and 80% in comparison to PBR without static mixers (Cheng et al., 2014; Yan, Guan, Jia, Huang, & Yang, 2018; T. Zhang, 2013).

Due to the above, we proposed a static mixer inside the PBR, allowing to improve agitation, mixing, and LD cycles. Then, it was evaluated and modelled the agitation effect over global productivity of the reactor.

2.2 Agitation and mixing in PBR

An adequate mixing of the microalgae culture medium in PBRs helps prevent the formation of sediments, increases mass transfer, improves the interaction between coexisting phases and helps to the illumination distribution (Cheng et al., 2014). For those reasons mentioned previously, the mixing process has shown to have a great influence on the yield obtained in microalgae cultures (Huang et al., 2015). This has caused that mixing is taken into account as an important factor for process design in PBR. In this project, it was studied the effect of a static mixer on PBRs. This mainly due to the fact that in recent reports of the literature it has been demonstrated that they are an effective method to increase the degree of mixing in the suspension of microalgae (Huang et al., 2015).

Cheng and colleagues in their 2014 report (Cheng et al., 2014) presented a new design of tubular reactor with baffles located obliquely with several perforations. This design showed good performance in the mixing of the fluid and for the average velocity in the direction of illumination. This type of mixers promotes the circulation of cells between dark and illuminated areas, improving the LD cycles, this fact is of great value when it is designed a new tubular reactor. Figure 2-1 shows a representative diagram of the mixer proposed by Cheng. There, it is possible to see the geometry of the mixers, those are located at a distance from the entrance to the system, the two baffles form an angle between them, and they have a perforated area, which allows not only that the flow surrounds the obstacle, but also a part of it crosses the mixers.

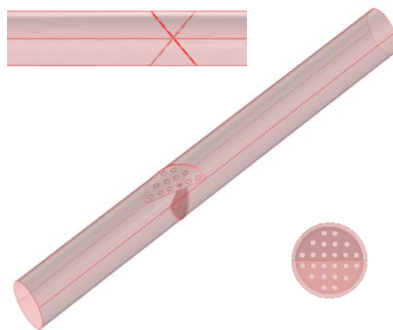


Figure 2-1: Diagram of the reactor for the simulation.

The mixer proposed by Cheng (Cheng et al., 2014) at the simulation level showed good results for fluid dynamics, however the pressure drops generated in the system due to the effect of this mixer achieve high values (114,755 Pa/dm), in comparison to the benefit that they can generate in productivity. Due to the above, some authors in the last years have taken into account not only the adequate mixing but also the energy consumption for the pumping system. For example: Gomez and colleagues studied CFD simulation of wall turbulence promoters, calculating energy consumption for the system (Gómez-pérez et al., 2015) in order to reduce energy consumption.

2.3 Mixer proposed and CFD simulation

In this subsection it is presented our new proposal of static mixer, as well as the CFD simulation and the performance of the agitation and mixing degree. Additional details and

calculations for the mixer proposed are presented in our research product (Salguero-rodríguez, Gómez-perez, José, & Oviedo, 2017). This subsection is organized as follows:

- First, it is presented the turbulence model as well as simulation parameters.
- Second, it is described the swirl number. This parameter is used to measure the mixing degree in the system.
- Finally, it is presented the new static mixer proposed in this thesis also the results regarding to mixing degree, velocities and hydrodynamic conditions.

2.3.1 Turbulence model

In this thesis it is studied the agitation and mixing performance of a new static mixer, in order to do that we simulated transport equations using the turbulence model $\kappa - \varepsilon$. The model was solved using COMSOL, a commercial program to perform CFD analysis.

The turbulence model $\kappa - \varepsilon$, is one of the most used for industrial applications, this model considers transport equations related to the kinetic energy of turbulence, κ , and the energy dissipation rate, ε . COMSOL models the viscosity μ_T with (2-1), in which C_μ represents a model constant. The transport equation for κ is shown in (2-2).

$$\mu_T = \frac{\rho C_\mu \kappa^2}{\varepsilon} \quad (2-1)$$

$$\rho \frac{\partial \kappa}{\partial t} + \rho \mathbf{u} * \nabla \kappa = \nabla * \left(\left(\mu_d + \frac{\mu_T}{\sigma_\kappa} \right) \nabla \kappa \right) + P_\kappa - \rho \varepsilon \quad (2-2)$$

Where the term P_κ is given by (2-3). The transport equation for ε is shown in (2-4). In those equations ρ represents the density of the fluid, \mathbf{u} the average velocity, t the time, μ_d the dynamic viscosity, P the pressure, κ the turbulence energy, ε the dissipation of turbulence energy.

$$P_\kappa = \mu_T \left(\nabla \mathbf{u} * (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} (\nabla * \mathbf{u})^2 \right) - \frac{2}{3} \rho \kappa \nabla \mathbf{u} \quad (2-3)$$

$$\rho \frac{\partial \varepsilon}{\partial t} + \rho \mathbf{u} * \nabla \varepsilon = \nabla * \left(\left(\mu_d + \frac{\mu_T}{\sigma_\varepsilon} \right) \nabla \varepsilon \right) + C_{\varepsilon 1} P_\kappa - \frac{C_{\varepsilon 2} \rho \varepsilon^2}{\kappa} \quad (2-4)$$

Parameters of those models are determined through experimental work; an example of those values are presented in the COMSOL manual. Those are shown in the table 2-1 (COMSOL, 2012).

Table 2-1: Model parameters turbulence model.

Taken from COMSOL Manual (COMSOL, 2012).

Parameter	Value
C_{μ}	0.09
$C_{\varepsilon 1}$	1.44
$C_{\varepsilon 2}$	1.92
σ_{κ}	1.0
σ_{ε}	1.3

Once it is simulated the turbulence model in COMSOL, results can be exported to other programs for later processing such as: Microsoft Excel, Matlab. In this thesis, it was quantified mixing degree using a metric proposed in the literature, it is shown in the next subsection. The mixing degree was calculated with the velocity profile previously computed in COMSOL.

2.3.2 Swirl number

Swirl number (Sn) has been used as a good criterion in order to establish the mixing performance of the PBR (L. B. Wu, Li, & Song, 2010). This dimensionless number represents the relationship between angular and axial momentum (Q. Zhang, Wu, Xue, Liang, & Cong, 2013).

Swirl number has been used to quantify the degree of mixing achieved in the PBR reactors (L. B. Wu et al., 2010), the expression to calculate the swirl number in the cross-sectional area of the reactor is shown in (2- 5).

$$Sn = \frac{\iint UVrdS}{\iint U^2rdS} \quad (2-5)$$

Where U represents the average axial component of the velocity; V is the circumferential component of the velocity; r is the radial distance, and S is the cross section under study. In Figure 2-2, those variables are shown in the cross-sectional area of a cylinder.

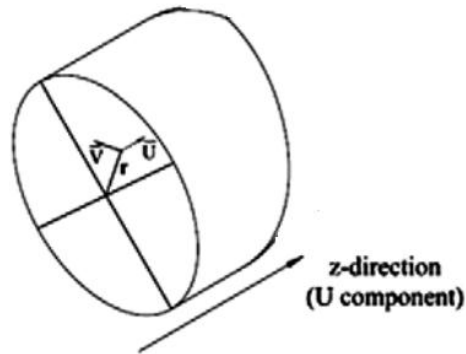


Figure 2-2: Cross-sectional area of the PBR.
Taken from Wu et al. (L. B. Wu et al., 2010).

2.3.3 Static mixer proposed

As it was shown previously, not only it is important to promote LD cycles inside the PBR through and adequate mixing degree, but also taking into account that an excessive mixing degree will increase energy consumption for the system. Due to the above, another type of mixer was proposed in this work, which fulfilled the objective of promoting an adequate mixing inside the reactor and an oscillation of the microalgae between illuminated and dark areas. The proposed new mixer is shown in Figure 2-3, this is composed by two crossed baffles, located with a relative angle of 90° the right baffle with respect to the left, and with this change it was possible to reduce the pressure drop in the PBR in comparison to other static mixers, as the presented previously by Cheng (Cheng et al., 2014).

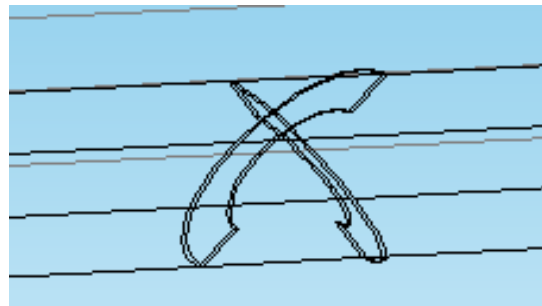


Figure 2-3: Static mixer proposed for the PBR.

The turbulence model was simulated in COMSOL with the boundary conditions shown in (2-6). Where V_a , represents the average velocity normal to the flow area and P_{atm} is the atmospheric pressure; the last condition to fulfill the continuity equation.

Input $u = V_a$,

Output $P_{out} = P_{atm}$ (2-6)

Wall $u = 0$,

Firstly, it was necessary to simulate the tubular reactor without any flow obstacle, this in order to be able to establish a later comparison between hydrodynamic conditions of the system with or without static mixers. Figure 2- 4 shows the study geometry used for the simulation of the photobioreaction system in COMSOL, the shape of the reactor was a cylinder with a radius of 0.025 m and a total length of the cylinder of 2 m was used. Those parameters were taken from values suggested in the PBR literature previously presented. Total length was adjusted to avoid excessive computation time for the model.

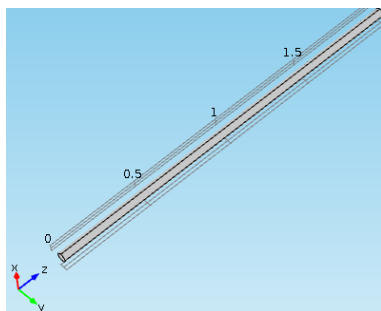


Figure 2-4: Geometry of the PBR without mixers.

Figure 2-5 shows the velocity and pressure drop profile in the PBR without mixers with a linear velocity of 0.3 m/s, in which it is noticeable that the vicinity of the walls of the reactor are at low velocities, while the central part approaches a maximum velocity, it is also evident that the velocity profile changes its behavior until it is established at a length close to 12.5% of the total length, which corresponds to 0.25 m. The total pressure drop for the system with the velocity previously mentioned corresponded to approximately 54.3 Pa in the total length of the cylinder, it means 2.715 Pa/dm. This is the pressure drop of the system without static mixers, any flow obstacle inside the reactor will increase the pressure drop. As it was highlighted previously, the main idea to improve the agitation in this system is to promote LD cycles and at the same time avoid excessive energy consumptions in the system.

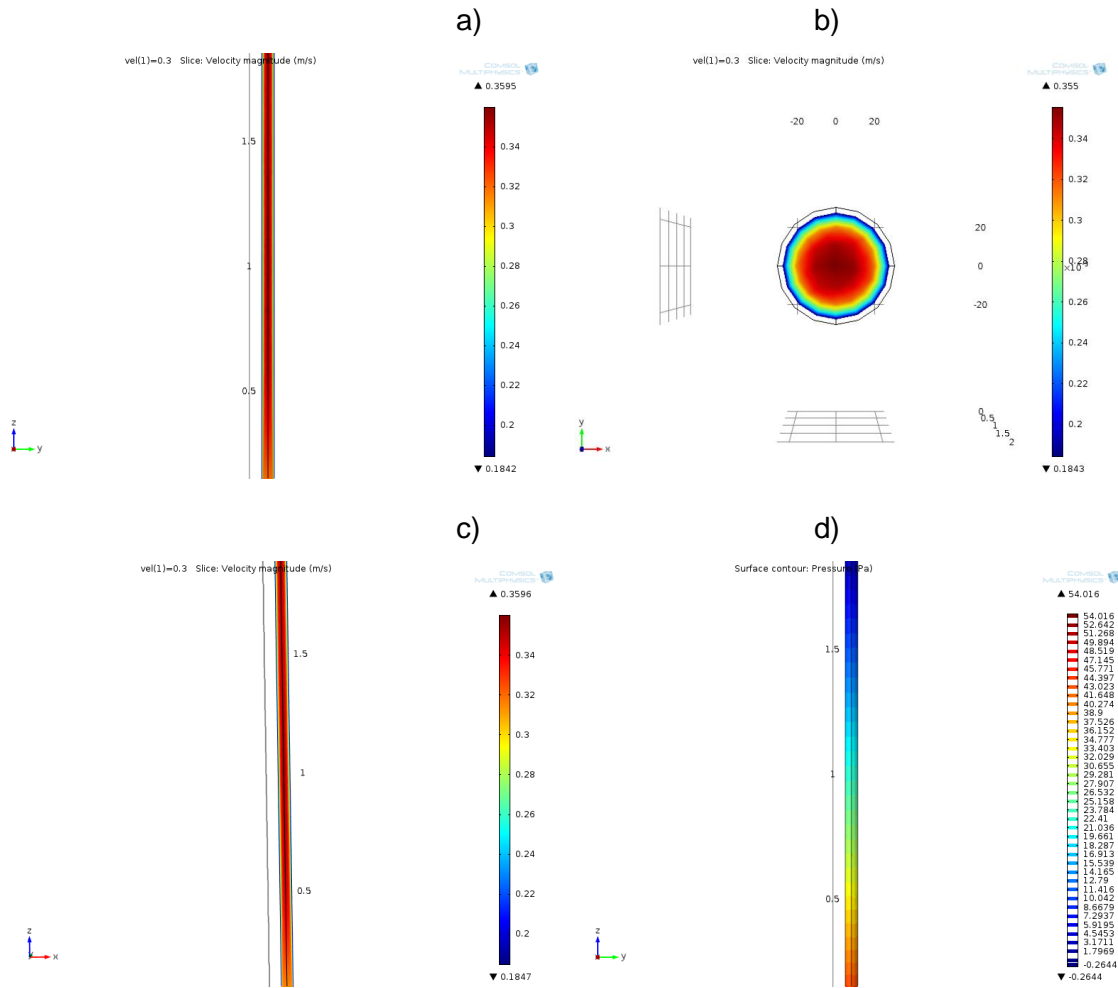


Figure 2-5: Profiles for the reactor without mixer a) velocity z-y view b) velocity x-y view c) velocity z-x view d) pressure drop

Figure 2-6 shows the study geometry used for the simulation of the photobioreaction system in COMSOL, for this purpose it was used a cylinder with a radius of 0.025 m, inside the cylinder the mixer with crossed baffles was located, at a length of 0.25 m, which corresponds to approximately 12.5% of the total length of the cylinder of 2 m, this initial length allows to guarantee that the flow profile before reaching the mixer is fully developed.

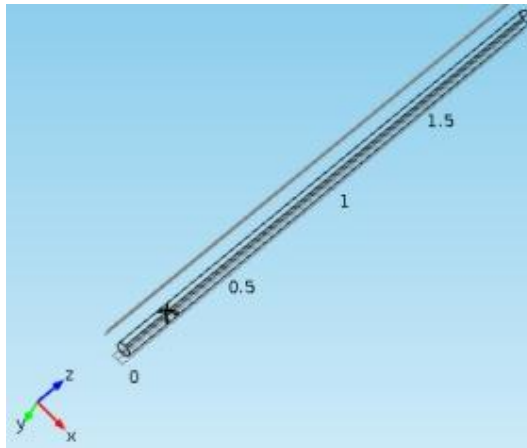


Figure 2-6: Study geometry used in COMSOL with static mixer.

The results showed by Perner in his publication (Perner-Nochta & Posten, 2007), suggest that with velocities of 0.5 m/s good growth rates and product concentrations are obtained in a reactor without external mixing conditions, so it is expected that when using a mixer in the system this flow rate can be reduced, without negatively affecting the microalgae. To perform this simulation, the turbulent flow module and the particle tracking module were used, with a nominal velocity located in the range of 0.1 m/s to 0.5 m/s. The results for a static mixer are shown in Figure 2- 7, where it is possible to appreciate the velocity profile and pressure drop. In the velocity profile, it is clear that the mixer increases the average velocity of the fluid from a value close to 0.3 m/s to 0.59 m/s, it means that the velocity practically is duplicated. The total pressure drop in the reactor is 185.92 Pa, which represents an average of 9.26 Pa/dm, this value is lower than the value mentioned for the Cheng mixer.

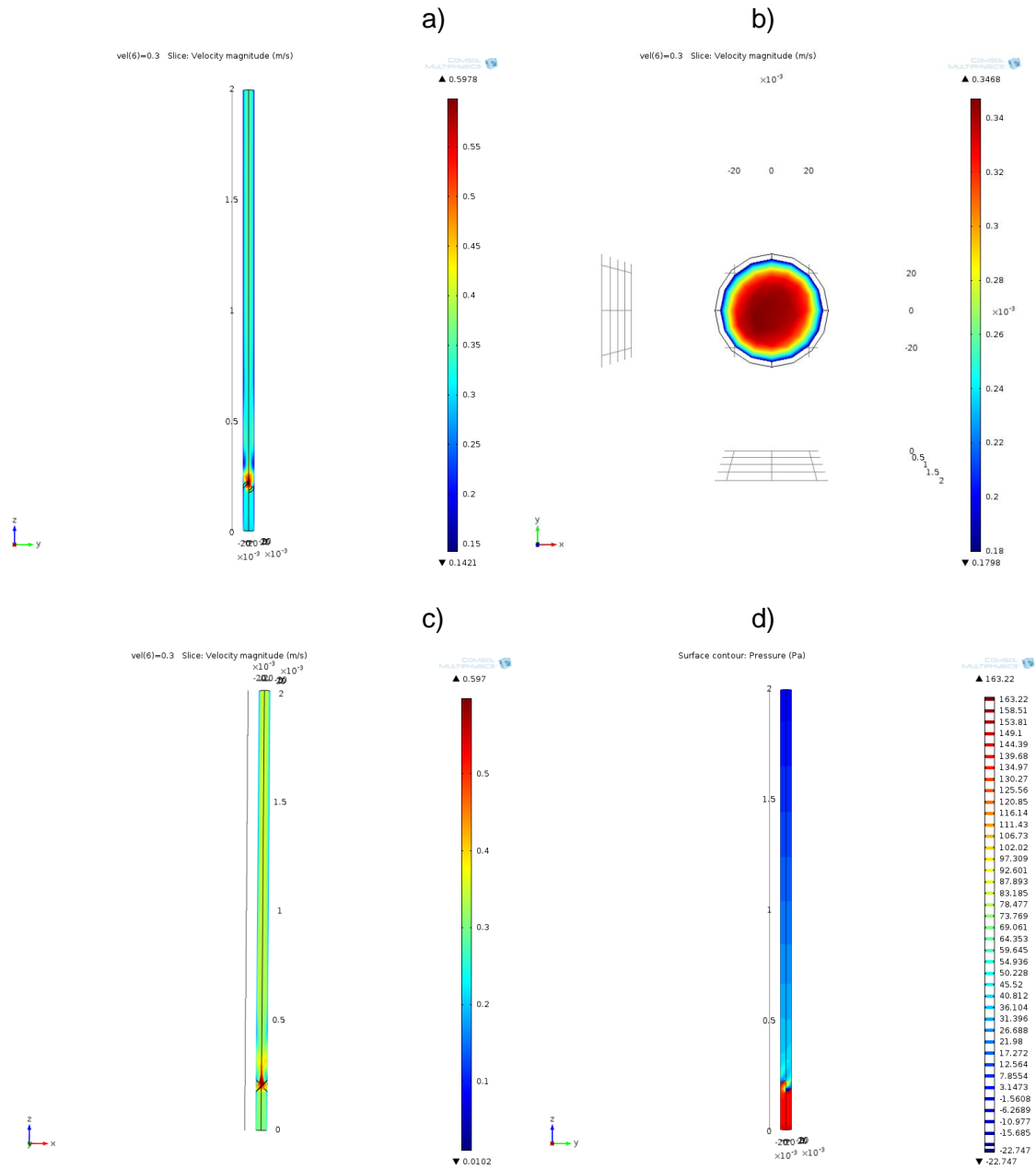


Figure 2-7: Profiles for the reactor with one static mixer a) velocity z-y view b) velocity x-y view c) velocity z-x view d) pressure drop

To establish the effect on the mixing of the proposed static mixers, the swirl number was calculated after 1 dm in the reactor of 2 m of total length. Similarly, in order to establish the relationship of the average linear velocity of the culture and the achieved mixing, the dynamics of the fluid were simulated with different velocities from 0.1 m/s to 0.5 m/s, those results are shown in Figure 2-8.

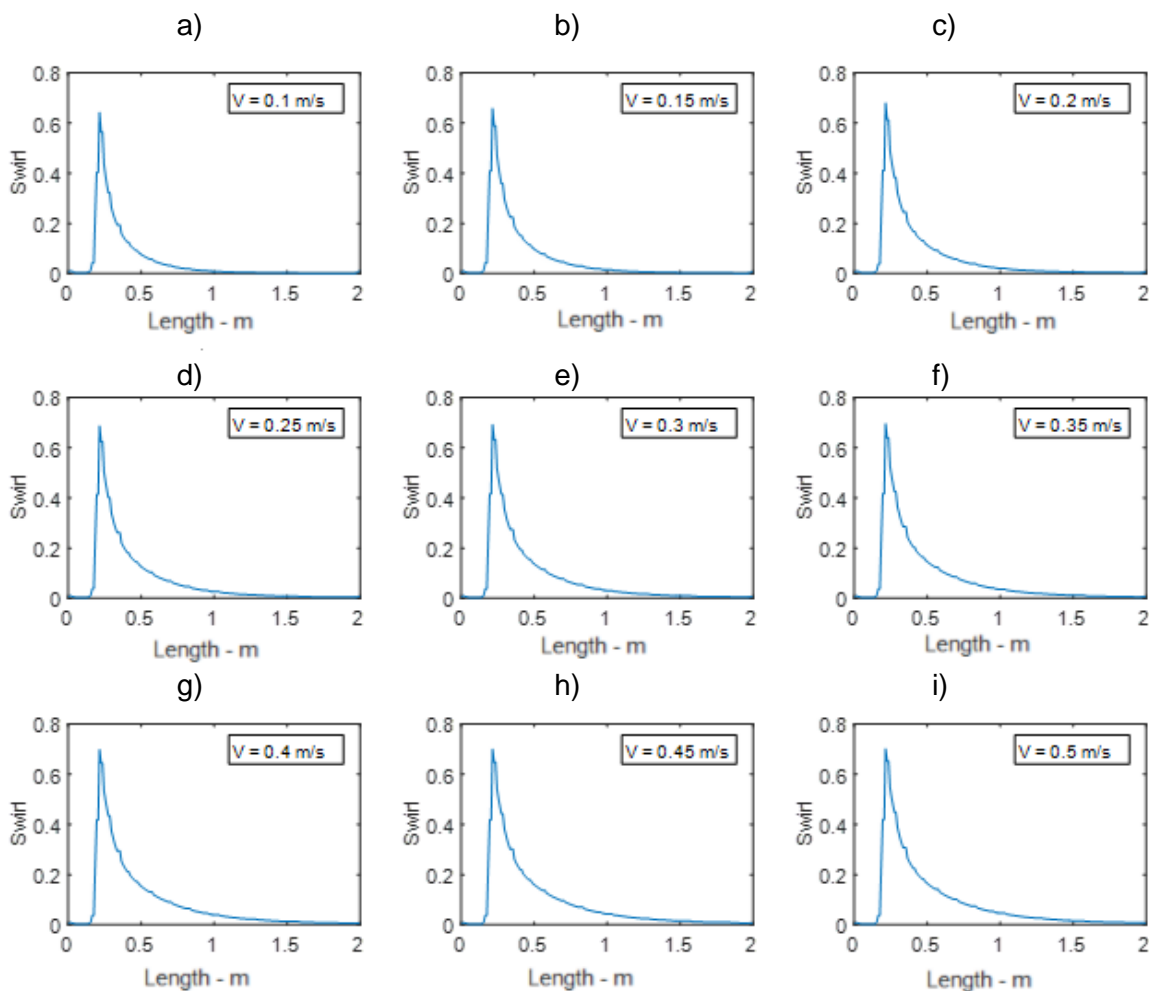


Figure 2-8: Swirl number profile as a function of length for various linear velocities using one static mixer a) 0.1 m/s b) 0.15 m/s c) 0.2 m/s d) 0.25 m/s e) 0.3 m/s f) 0.35 m/s g) 0.4 m/s h) 0.45 m/s i) 0.5 m/s.

In the results obtained for the mixing degree, it is important to note that as the average linear velocity increases, the maximum value reached for this parameter increases in the same way. It is also evident that, with a higher velocity, the disturbance introduced into the system by the mixer sustains the swirl number with values higher than 0.1 for a longer length. The effect of the mixer is able to maintain the mixing of the culture for all the velocities approximately a length of 50 cm, due to it, this length was chosen as minimum spacing of the mixers.

Figure 2-9 shows the velocity profile for two mixers, in the first case located at a distance of 50 cm, and in the second located at a distance of 80 cm, the velocity profiles show similar values in both cases. The pressure drops reached by both configurations are very similar, so they are not taken into account as a criterion for the selection of the best configuration.

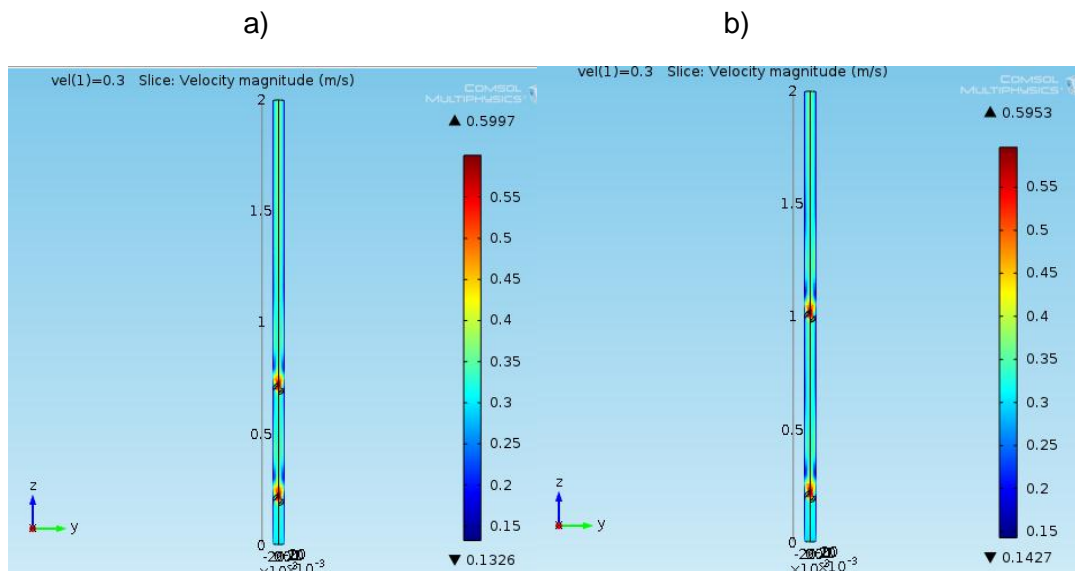


Figure 2-9: Velocity profile with different spacing a) 50 cm b) 80cm

In Figure 2-10 is shown the swirl number profile for two mixers, in the first case located at a distance of 50 cm, and in the second located at a distance of 80 cm, for the shortest distance is the best mixing, due to the fact that the degree of mixing is maintained at higher values for a longer length, and always with a value greater than 0.1 for the swirl number. Therefore, the spacing between mixers is chosen as 50 cm.

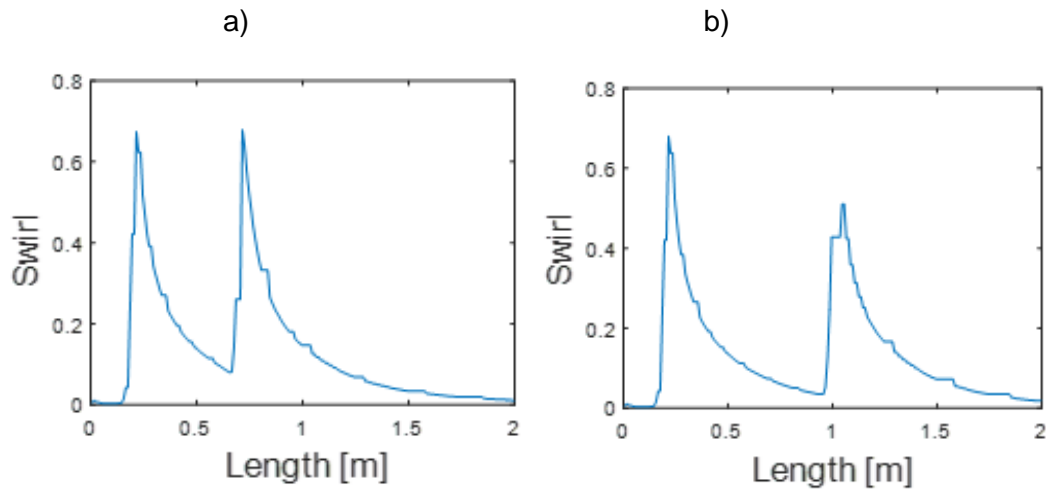


Figure 2-10: Profile swirl number with different spacing a) 50 cm b) 80cm.

Taking into account the profiles shown for the swirl number, the pressure drops and the average speed reached by the fluid, the most favorable conditions for the culture result with a spacing between the mixers of 50 cm. Figure 2-11 shows the geometry study, for a cylindrical reactor with 4 mixers, with a spacing of 50 cm between them; the first one located 0.25 m from the beginning of the pipeline and the last one located 0.25 m from the end of the pipeline.

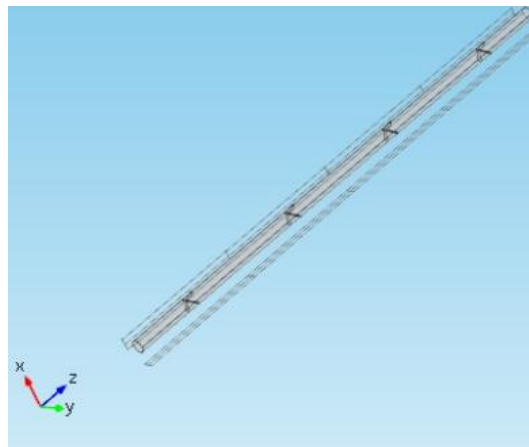


Figure 2-11: Geometry of the reactor with four mixers.

Figure 2-12 shows the profile of the velocity and pressure drop obtained with the configuration of 4 mixers. The velocity rises to 0.59 close to the mixer, effect of the reduction of the flow area, and velocity has low values near to the walls of the reactor. The total

pressure drop for the system is 484.901 Pa, which represents an average pressure drop of 24.245 Pa / dm.

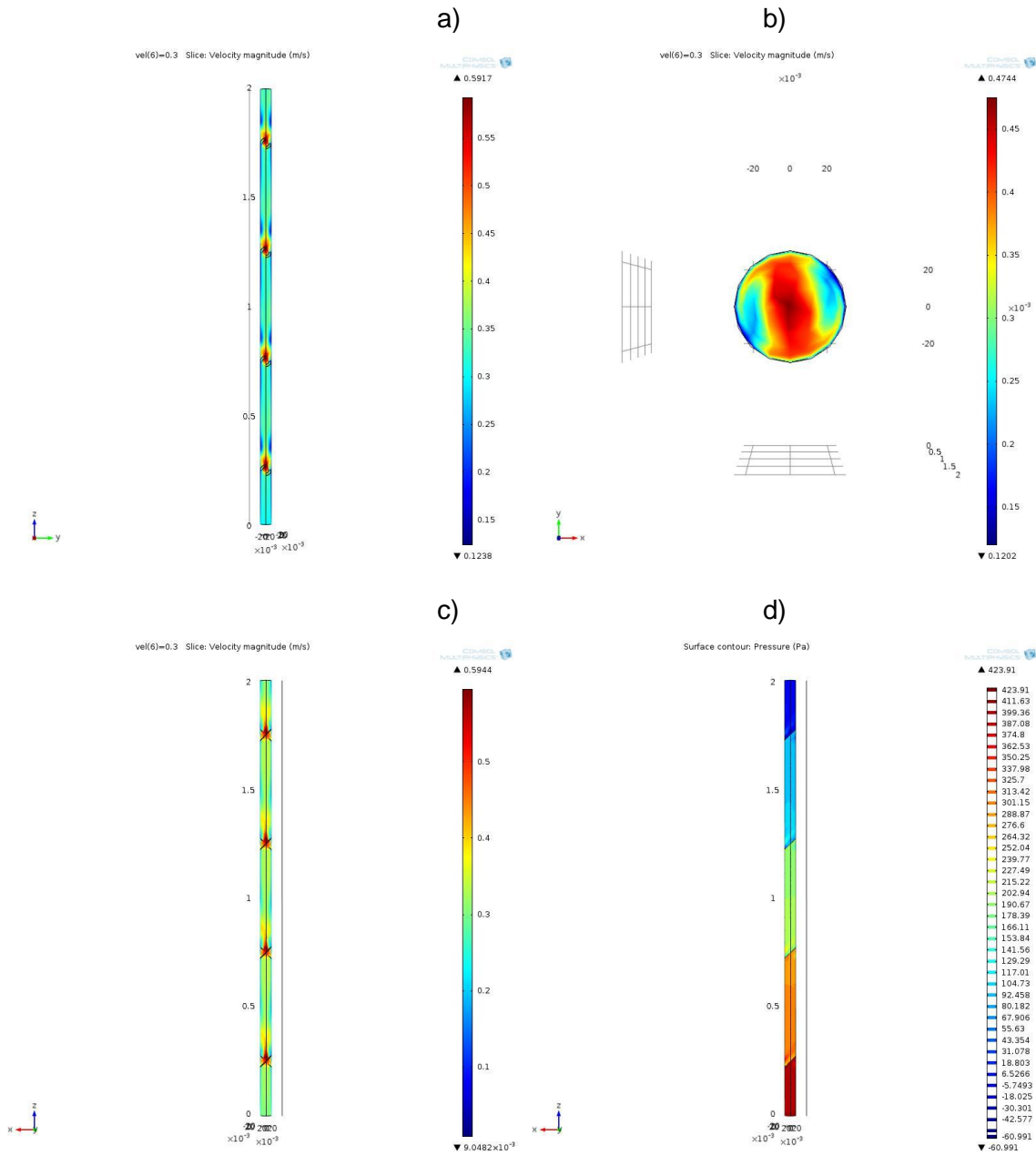


Figure 2-12: Profiles for the reactor with four static mixers a) velocity z-y view b) velocity x-y view c) velocity z-x view d) pressure drop

Figure 2-13 illustrates the value of the swirl number along the reactor, it is shown that it rises to its maximum value in the mixer coordinate, and it decreases to a value close to 0.1 in the 50 cm of spacing. It is important to note that from the first mixer the number of swirl

in the whole pipe is maintained with values above 0.8 which indicates that even the areas away from the mixer have an adequate degree of mixing.

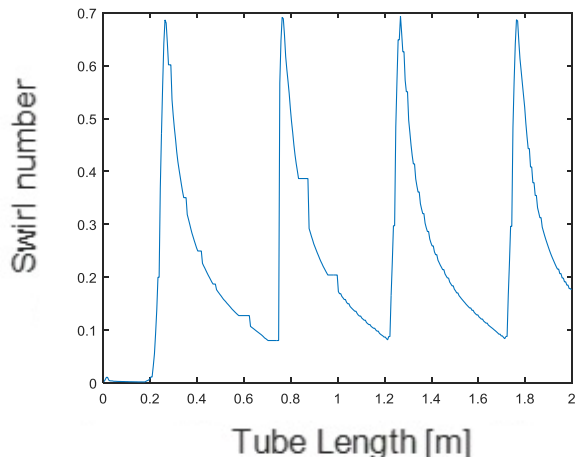


Figure 2-13: Swirl number profile for some static mixers.

The mixer proposed in this work lets microalgae culture achieve a good mixing degree without dramatic energy consumption in contrast to some mixers presented in the literature. As it was mentioned previously, mixing helps LD cycles inside the culture, and as a result productivity is improved. After it is established the static mixer and the hydrodynamic conditions for the culture, it is thus necessary to model the effect of it on the productivity of the PBR. The next chapter presents the model of the PBR taking into account the static mixer proposed as well as the LD cycles effect.

It is important to note that for further steps it could be useful to study the effect of velocity and the shape of the mixer in relation to the cell stress and shear stress.

Chapter 3: Dynamic model of the photobioreactor

This chapter shows a new dynamic model for photobioreactor control, which can predict the effect of agitation and light-dark cycles on productivity of the culture. This sections is presented as follows:

- Firstly, it is shown the modelling of the photobioreactor, models used from the literature such as: illumination model, growth kinetics model as well as our own results for parameters.
- Finally, it is presented the main results regarding to dynamic performance of the photobioreactor using the new proposed model.

3.1 Modelling of the photobioreactor

In this section, it is presented a dynamic model of the PBR. It is a new model that allows to take into account the effect of LD cycles, agitation, mixing on the productivity of the system. According to previous studies those are the variables that show high impact on the economy of this process. This new model takes into account the following phenomena: hydrodynamic inside the reactor, agitation and mixing degree, kinetic growth, LD cycles effect and the effects of different disturbances of the model such as: external illumination and biomass initial concentration.

This section is organized as follows:

- Description of the tubular PBR: it is necessary to understand the operation of the equipment, and the phenomena that take place inside it for an adequate model.
- Photobioreactor model: once the PBR and the mixer to be used are established, it is necessary to establish the model that allows to represent the behavior of the light-dark cycles. The model of LD cycles is always dynamic in the system, due to it, the PBR model has to be dynamic.

- Kinetics of photosynthesis for microalgae: the dynamic model of the PBR requires the specific growth rate of microalgae. Therefore, it is necessary to couple a kinetic model, in this case it was the model of three states of the Photosynthetic Unit - PSU.
- Illumination simulation: it is necessary to represent the illumination as a function of the agitation in the system. It allows to predict the growth behavior of the microalgae with the LD cycles.

3.1.1 Description of the Photobioreactor

The PBR can be divided into two main parts. In the first section is found the solar receiver, which is designed to maximize the capture of solar radiation, minimizing the resistance to flow and occupying the smallest area as possible. In the second section, there is a bubble column, which is used to mix, degas and supply energy to the culture. Further details about the modeled system can be found in Fernández and colleagues publication (Fernández et al., 2014) and Molina et al. (Molina et al., 2001), in which the operation of all of them is explained in high detail. Besides of that, the dimensions and parameters are shown in those papers. Figure 3-1 shows a representative diagram of the PBR.

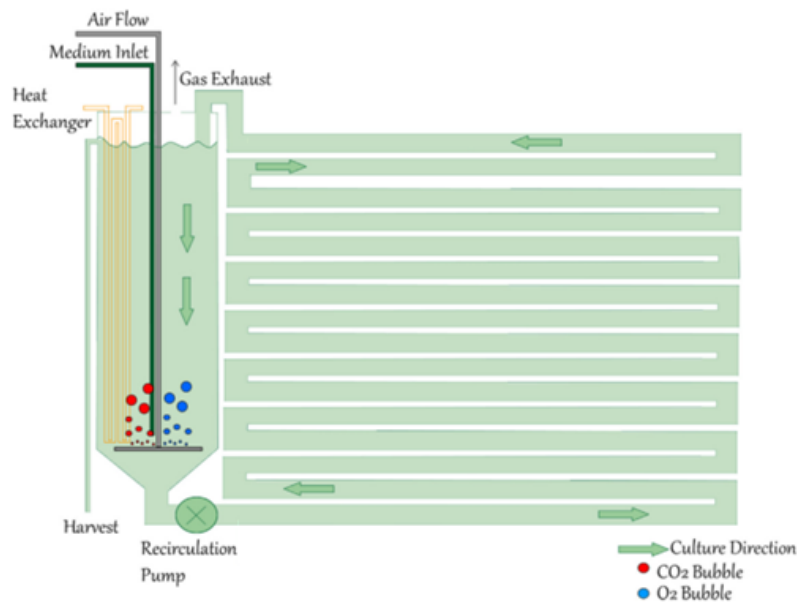


Figure 3-1: Diagram of the PBR.

Taken from Fernández (Fernández et al., 2014).

In order to study the productivity of the system, the model focus on the solar receiver section. In Figure 3-2, the diagram of the PBR is shown, in which the solar receiver is highlighted. For purposes of modelling, the area of the solar receiver can be divided into n sections, where each of those represents a section of the pipeline, and where the output of each subsystem is the input of the next subsystem.

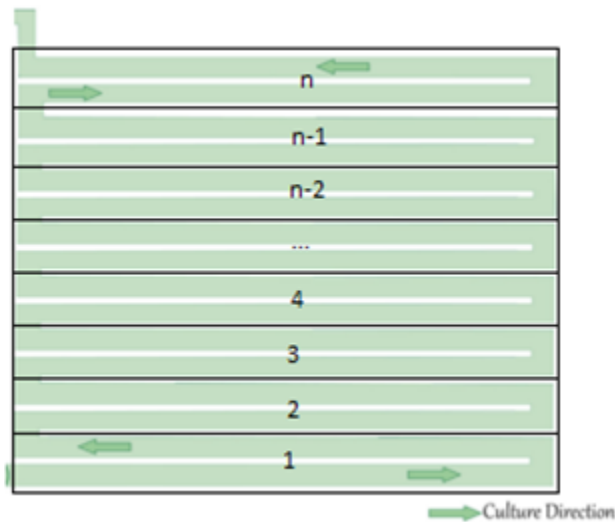


Figure 3-2: Diagram of the solar receiver.

Adapted from Fernández (Fernández et al., 2014).

In Figure 3- 3, it is presented the process system diagram in which the solar receiver is divided using n sections. The initial element, which it is denoted by 1, then we have a mass flow F_i , with a mass concentration of carbon dioxide C_{iCO_2} , a mass concentration of oxygen C_{iO_2} , and a mass concentration of biomass C_{ib} . The output of the first element corresponds to the input of the second element, and consequently, the output of the element $n-1$ is the input of the final element n . The subindex under each of the variables denotes the element of the solar receiver associated.

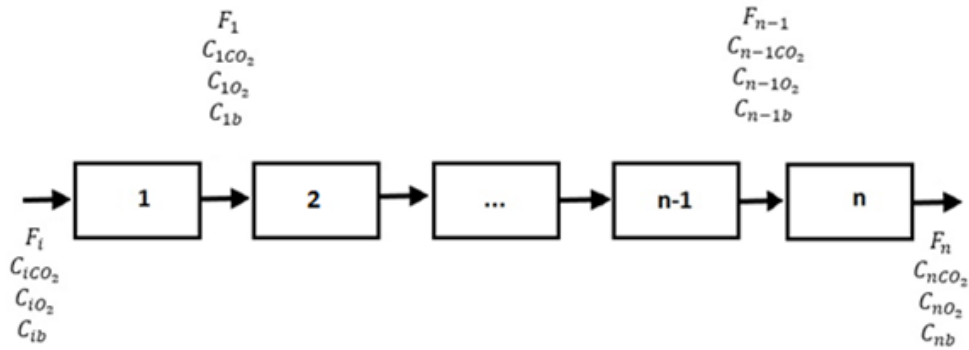


Figure 3-3: Diagram of the solar receiver divided into sections.

3.1.2 Dynamic model of the photobioreactor

The model to be presented has implicit the following assumptions:

- Mass transfer in the bubble column is efficient, due to this fact, it is presumed that saturated CO_2 in aqueous solution is fed to the receiver, it means, the maximum possible dissolved amount of carbon.
- Heat exchange system has control actions that allow to maintain a uniform and constant temperature in the PBR, because of that, it is assumed constant and its effect is not modeled in the system.
- Oxygen concentration in the system at any point is equal or less than the saturation of the medium.
- System has a homogeneous phase, without the presence of different phases.
- Fluid density with low variations. It is approximately constant.

The variables of interest in this system are the concentration of the biomass, and the chemical species involved in photosynthesis such as CO_2 and O_2 . When performing the material balance for each of the variables, together with the global material balance in the initial element, denoted as i in the subindex, the expressions from (3-1) to (3-4) are obtained.

$$\frac{dM_{1sis}}{dt} = F_i - F_1 \quad (3-1)$$

$$\frac{dM_{1CO_2}}{dt} = \frac{1}{\rho} F_i C_{iCO_2} - \frac{1}{\rho} F_1 C_{1CO_2} - \gamma_{1CO_2} \quad (3-2)$$

$$\frac{dM_{1O_2}}{dt} = \frac{1}{\rho} F_i C_{iO_2} - \frac{1}{\rho} F_1 C_{1O_2} + \gamma_{1O_2} \quad (3-3)$$

$$\frac{dM_{1b}}{dt} = \frac{1}{\rho} F_i C_{ib} - \frac{1}{\rho} F_1 C_{1b} + \gamma_{1b} \quad (3-4)$$

Where the total mass of the element analyzed is M_{1sis} in g and the mass of the carbon dioxide, oxygen and biomass are represented by M_{1CO_2} , M_{1O_2} and M_{1b} in g. The reaction rates for carbon dioxide, oxygen and biomass are represented by γ_{1CO_2} , γ_{1O_2} , γ_{1b} in g/s. The mass flows F_i and F_1 in g/s, with a mass concentration of carbon dioxide C_{iCO_2} in g/l, a mass concentration of oxygen C_{iO_2} in g/l, and a mass concentration of biomass C_{ib} in g/l.

Assuming that the fluid density presents low variations; it means approximately constant. It is possible to establish that in the system there is not net accumulation of mass. It is possible to simplify the global material balance as indicated in the expression (3-5).

$$F_i = F_1 \quad (3-5)$$

For simplification purposes, it is assumed that the agitation achieved in the system is capable of maintaining homogeneous conditions. Therefore, the properties inside the analyzed element corresponds in an equivalent way to the values of the properties at the output of the same. The mass of carbon dioxide in the system can be evaluated with (3-6).

$$M_{1CO_2} = V_1 P_{CO_2} [CO_2]_1 \quad (3-6)$$

where, P_{CO_2} is the molecular weight of CO_2 in g/mol, V_1 is the volume of the system in l and $[CO_2]_1$ is the molar concentration of carbon dioxide in mol/l.

In the fixation of a CO_2 molecule and subsequent transformation in the photosynthetic process, 4 electrons are required for each molecule that is fixed. For this, 8 photons of visible radiation are required to raise the potential energy of the 4 electrons of the water in the two photosystems that work in series (Jaramillo & Bustamante, 2005). In that order of ideas, the global equation for photosynthesis can be written as shown in (3-7). Taking into account that the stoichiometric ratio for carbon dioxide and oxygen is 1: 1, we can say that their reaction rates, on a molar basis, will be equivalent, as shown in (3-8).



$$\gamma_{CO_2} = \gamma_{O_2} \quad (3-8)$$

The molar velocity term for the consumption of carbon dioxide and appearance of oxygen are related to the growth kinetics of microalgae, and at the same time to the stoichiometry of the photosynthetic reaction. First we can establish a molar ratio of 1:8 for the amount of carbon dioxide and oxygen in the reaction and the photons used, when expressing them as grams we have the expressions (3-9) and (3-10).

$$\frac{1 \text{ mol } CO_2}{8 \text{ mol } hv} = \frac{44 \text{ g } CO_2}{8 \text{ mol } hv} = 5.5 \frac{\text{g } CO_2}{\text{mol } hv} \quad (3-9)$$

$$\frac{1 \text{ mol } O_2}{8 \text{ mol } hv} = \frac{32 \text{ g } O_2}{8 \text{ mol } hv} = 4 \frac{\text{g } O_2}{\text{mol } hv} \quad (3-10)$$

An approximate composition of microalgae in mass percentage is 70% in carbon (Zijffers, Schippers, Zheng, Janssen, & Tramper, 2010), it is possible to make an equivalence between the fixed carbon and the amount of biomass in the system, according to the expressions (3-11) and (3-12).

$$\frac{1 \text{ mol } C \text{ fixed}}{8 \text{ mol } hv} = \frac{12 \text{ g } C}{8 \text{ mol } hv} = 1.5 \frac{\text{g } C}{\text{mol } hv} \quad (3-11)$$

$$1.5 \frac{\text{g } C}{\text{mol } hv} \times \frac{1 \text{ g biomass}}{0.7 \text{ g } C} = 2.14 \frac{\text{g biomass}}{\text{mol } hv} \quad (3-12)$$

The mass velocity of carbon dioxide consumption can be considered independent of its concentration. It can be assumed because the system has enough amount of carbon dioxide for the photosynthesis reaction shown in (3-7). On the opposite, the illumination can generate dark areas and photoinhibition as a result of the high concentrations of biomass used frequently. Due to it, the illumination is considered as the limiting factor of this reaction, which influences the specific growth rate (μ) through kinetic models. The stoichiometry of the reaction and the specific growth rate achieved under the illumination regime are related to the rate of dioxide consumption in (3-13). The mass velocity of oxygen is shown in equation (3-14).

$$\gamma_{1CO_2} = V_1 \mu C_{1b} \times \frac{5.5 \text{ g } CO_2}{2.14 \text{ g biomass}} \quad (3-13)$$

$$\gamma_{1O_2} = V_1 \mu C_{1b} \times \frac{4 \text{ g } O_2}{2.14 \text{ g biomass}} \quad (3-14)$$

Where V_1 is the volume of the system in l, C_{1b} is the mass concentration of biomass in the study element in g/l, μ is the growth rate in 1/s, γ_{1CO_2} is the rate of dioxide consumption in g/s and γ_{1O_2} is the rate of oxygen appearance in g/s.

It is possible to rewrite the biomass in the system as the product, between the volume and the concentration of biomass, as it is shown in the expression (3-15). The mass velocity of appearance of the biomass can be represented by (3-16).

$$M_{1b} = V_1 C_{1b} \quad (3-15)$$

$$\gamma_{1b} = V_1 \mu C_{1b} \quad (3-16)$$

Where V_1 is the volume of the system in l, C_{1b} is the mass concentration of biomass in the study element in g/l, M_{1b} is the mass of biomass in g, μ is the growth rate in 1/s, γ_{1b} is the biomass reaction rate in g/s.

The term that accompanies the gradient of concentrations of both chemical species and biomass, it can be simplified taking into account that the mass flow divided by density is equivalent to the volumetric flow (\dot{V}_i) in l/s, which at the same time can be expressed as the product between the average flow velocity (v) in m/s and the cross-sectional area (A) in m². As the study elements represent cylinders, the volume of each element is given by the product between its area and the length of the element (L_1) in m. By simplifying this expression, it is obtained (3-17).

$$\frac{F_i}{V_1 \rho} = \frac{\dot{V}_i}{V_1} = \frac{vA}{AL_1} = \frac{v}{L_1} \quad (3-17)$$

By replacing the expressions (3-6), (3-13), (3-14), (3-15), (3-16) and (3-17) in the balances for carbon dioxide, oxygen and biomass expressions are obtained (3-18), (3-19) and (3-20), which allow to analyze the behavior of the PBR as a function of time. In this section, the analysis for the first differential element (number n=1) has been shown, but it is enough to change the subindex to analyze more than 1 element.

$$\frac{d[CO_2]_1}{dt} = \frac{v}{L_1} ([CO_2]_i - [CO_2]_1) - \frac{2.56\mu C_{1b}}{P_{CO_2}} \quad (3-18)$$

$$\frac{d[O_2]_1}{dt} = \frac{v}{L_1} ([O_2]_i - [O_2]_1) + \frac{1.866\mu C_{1b}}{P_{O_2}} \quad (3-19)$$

$$\frac{dC_{1b}}{dt} = \frac{v}{L_1} (C_{ib} - C_{1b}) + \mu C_{1b} \quad (3-20)$$

3.1.3 Kinetics of photosynthesis

In the model presented in the previous section, it is required to evaluate the growth kinetics of microalgae. Due to the above, it is necessary to evaluate a model for photosynthesis that

allows to take into account the LD cycles. Most of the existing kinetic models have been built based on the Photosynthetic unit - PSU. A PSU usually refers to the coupling of a chlorophyll molecule involved in the generation of an oxygen molecule or fixation of a molecule of carbon dioxide. This contains photosystems I and II (Han, 2001). In the literature the Photosynthetic factory - PSF and Photosynthetic unit - PSU models are presented, having the same meaning. In Figure 3-4, the basic diagram representing the kinetic models based on PSU is shown. The models based on PSU (Eilers & Peeters, 1988) contemplate three states, which are: X_1 state of rest; X_2 state activated and X_3 the state inhibited.

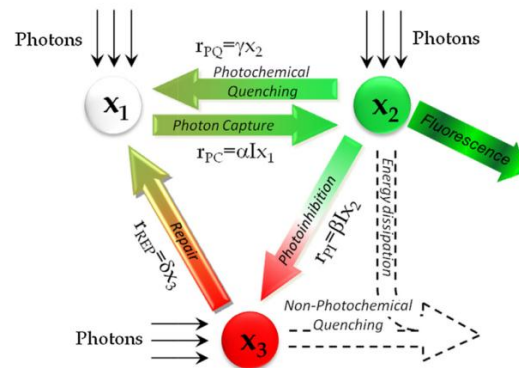


Figure 3-4: Schematic representation of kinetic models based on PSU.

Taken from Gargano (Gargano et al., 2015).

In publications of Wu and Merchuk during the penultimate decade (Merchuk & Wu, 2003; X. Wu & Merchuk, 2001, 2002) it was shown a modification to the original model proposed for the kinetics in PSF. In this model, the cultivation process can be seen as the result of four elements that occur simultaneously:

1. The capture of photons, the start of biochemical reactions and the synthesis of biomass. In terms of the PSF model, $X_1 \rightarrow X_2$ can be indicated.
2. Start of dark phase reactions, which do not need illumination. In terms of the PSF model, $X_2 \rightarrow X_1$ can be indicated.
3. Loss of photons due to excessive illumination (photoinhibition), which in terms of PSF is $X_2 \rightarrow X_3$.
4. Recovery of photon capture, which can be summarized as: $X_3 \rightarrow X_1$.

While steps 1 and 3 only occur in periods of exposure to light, steps 2 and 4 do not need light. The net growth rate is the result of the integration of the 4 steps mentioned. The expressions that represent this model are shown in the equations from (3-21) to (3-25).

$$\frac{dx_1}{dt} = -\alpha I x_1 + \gamma x_2 + \delta x_3 \quad (3-21)$$

$$\frac{dx_2}{dt} = \alpha I x_1 - \beta I x_2 - \gamma x_2 \quad (3-22)$$

$$\frac{dx_3}{dt} = \beta I x_2 - \delta x_3 \quad (3-23)$$

$$x_1 + x_2 + x_3 = 1 \quad (3-24)$$

$$\mu = k\gamma x_2 - Me \quad (3-25)$$

Where x_1, x_2, x_3 are the fractions of PSF in open, closed and inhibited states. The other parameters are constants with a certain luminous intensity, in table 3-1 are shown the values reported for this model by Wu and Merchuk (X. Wu & Merchuk, 2002).

Table 3-1: Parameters of the kinetic model.

Adapted from Wu (X. Wu & Merchuk, 2002).

Parameter	Unit	Value
k	dimensionless	3.65×10^{-4}
Me	s^{-1}	1.64×10^{-5}
α	$(\mu E m^{-2})^{-1}$	1.935×10^{-3}
β	$(\mu E m^{-2})^{-1}$	5.7848×10^{-7}
δ	s^{-1}	4.796×10^{-4}
γ	s^{-1}	1.46×10^{-1}

In some applications this model has shown to be useful in representing the relationship between fluid dynamics and growth velocity. The model can also predict the effect that the illumination history of the cells has on productivity, it means the LD cycles (X. Wu & Merchuk, 2001).

3.1.4 Illumination and light – dark cycles model.

In the models presented for photosynthesis, an illumination function is required to predict the growth of microalgae under the effect of LD cycles. Therefore, in this section an empirical function is constructed for the LD cycles as a function of the agitation. CFD was used, and subsequently an illumination simulation combined with particle tracking in the COMSOL software.

The movement of particles in a fluid was simulated using a Newtonian model, from Newton second law, shown in (3-26) which indicates that the net force in a particle is equivalent to its change in the linear moment in a frame of inertial reference (COMSOL, 2013). Where F_D represents the drag force (3-27) and F_g the gravitational force (3-28).

$$\frac{d(m_p v)}{dx} = F_D + F_g \quad (3-26)$$

$$F_D = \frac{m_p 18\mu}{\rho_p d_p^2} (u - u_p) \quad (3-27)$$

$$F_g = \frac{m_p g (\rho_p - \rho)}{\rho_p} \quad (3-28)$$

In those equations, u_p represents the velocity of the particle, u velocity of the fluid, g the gravitational acceleration, ρ_p is the density of the particle, ρ the density of the fluid, m_p the mass of the particle, d_p the diameter of the particle.

The illumination received by the system was calculated using an attenuation model presented in 2004 by Luo (Luo & Al-Dahhan, 2004), which it is a modification to Beer-Lambert's law that involves the presence of a non-transparent medium and the light absorption experienced by the cells, this is presented in equation (3-29). Where I_E represents the external illumination, d is the distance of the cells to the illuminated surface, k_w and k_x are the extinction coefficients for the water and the cells respectively, and finally C_b is the cellular concentration of biomass.

$$I = I_E * \exp[-(k_x * C_b + k_w) * d] \quad (3-29)$$

For simulation purposes, the values showed in Table 3-2 reported by Béchet (Béchet, Shilton, & Guieysse, 2013) and Luo (Luo & Al-Dahhan, 2004) were used.

Table 3-2: Parameters of the attenuation model.

Adapted from Béchet (Béchet et al., 2013) and Luo (Luo & Al-Dahhan, 2004).

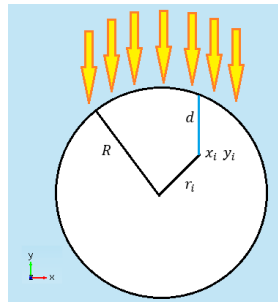
Parameter	Unit	Value
I_E	$\frac{\mu E}{m^2 s}$	450
k_w	m^{-1}	0.2
k_x	$\frac{ml}{m * cel}$	3×10^{-6}
C_b	$\frac{cel}{ml}$	8.0×10^6

The solar rays approach from a source located at a considerable distance from the surface of the PBR, for this reason, it can be assumed that their directions are parallel, and therefore the attenuation behavior is the same, presenting only changes in the relative location, due to the incidence of the sun. In Figure 3-5 the geometry is illustrated, where R represents the dimensions of the system, and any point located in the Cartesian coordinates has a radius r_i associated. Equation (3-30) represents the coordinates of the points that are on the surface of the system and equation (3-31) relates the coordinates of any point located inside the system with its radius r_i . To find the distance d, to the illuminated surface it is used the Pythagorean Theorem, which is shown in equation (3-32).

$$x^2 + y^2 = R^2 \quad (3-30)$$

$$x_i^2 + y_i^2 = r_i^2 \quad (3-31)$$

$$d = \sqrt{R^2 - x^2} - y_i \quad (3-32)$$

**Figure 3-5:** Cross-sectional area of the PBR

Once the simulation of computational fluid dynamics (CFD) with COMSOL was carried out, the particle tracking was simulated. To do this, the properties of a particle were configured

in the COMSOL interface, such as density, particle diameter among others. Figure 3-6 shows the trajectory on the vertical axis that follows a particle released in the velocity field for one of the low velocities, and one of the high velocities.

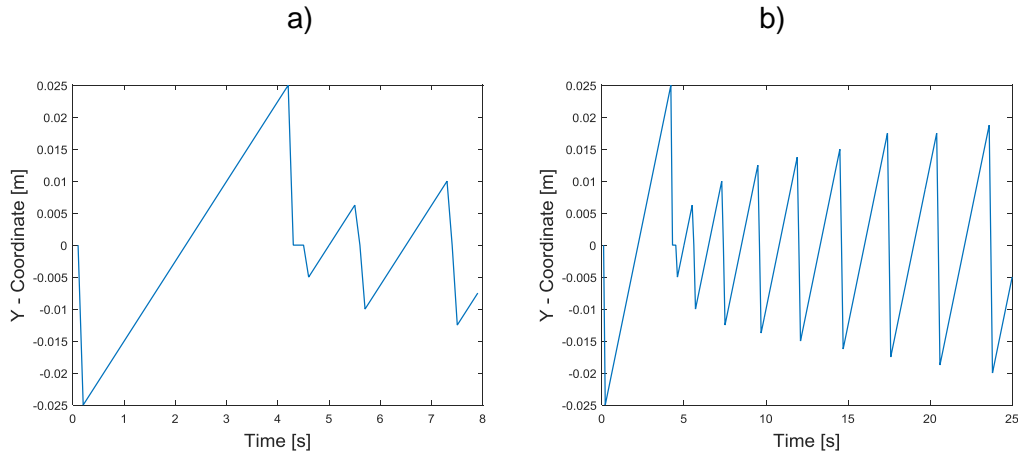


Figure 3-6: Trajectory on the vertical axis for a) $v = 0.55 \text{ m/s}$ b) $v = 0.1 \text{ m/s}$

The trajectories showed by this microalga, is an indicative of a periodic movement, however it is not perfectly equal throughout its trajectory. This is mainly due to the interactions with the other neighboring microalgae, which cause the trajectory to present some irregularities, it is also known that with a higher velocity, the particle experiences a greater number of cycles, that is, it has a greater frequency in its periodic movement. Figure 3-7 shows the results of the attenuation of the illumination in a cross-sectional area, the maximum values in the surface of the reactor are appreciable, of the order of $450 \mu E/m^2s$, and then those decrease as the depth increases in the reactor to a minimum value of $134.19 \mu E/m^2s$. Due to the above, the illumination that each of the particles can receive is between this range, and present variations according to the position of the microalgae.

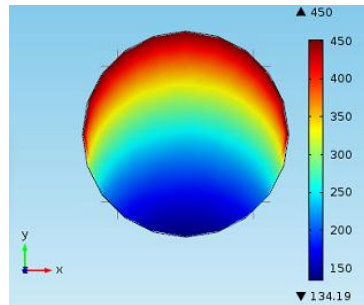


Figure 3-7: Illumination profile in the cross-sectional area PBR.

The illumination that a microalga experiences is shown in figure 3-8 for low and high velocities, it is noticeable that the illumination received by the microalga presents a behavior similar to that of the trajectory, in which it moves between the maximum and minimum illumination, and it repeats its behavior, with some irregularities, due to the interaction between the microalga and its neighboring particles. Similarly, it is known that with a higher velocity, the particle experiences a greater number of cycles, that is, it has a higher frequency in its periodic movement, and therefore it reduces its period of LD cycles.

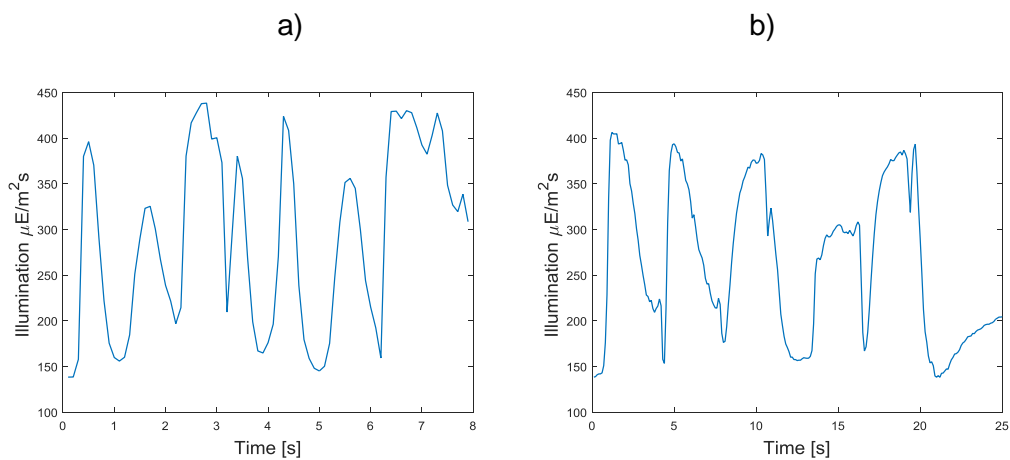


Figure 3-8: Illumination received by the microalgae. For a) $v=0.55$ m/s b) $v=0.1$ m/s

The particles are forced to experience an oscillatory movement, periodic in nature, it has associated one or several frequencies related to the number of oscillations that the particle can give in the unit of time. The Fourier transform allows to analyze the data of the illumination received by the particles in the frequency domain, where the presence of one or more dominant frequencies is more evident.

About 2000 particles were simulated in the system, so we have the same number of illumination profiles. Applying a window function for those profiles allows to analyze the set of profiles as a single profile, in which no discontinuities are perceived and therefore analyze in the frequency domain a unique profile for the system.

After applying the window function of the data to the illuminations, all the signals coming from each microalga in a single vector were concatenated, which was analyzed by means of the Fourier transform in the frequency domain. In Figures 3-9 a) and b) the signal are shown in the frequency domain.

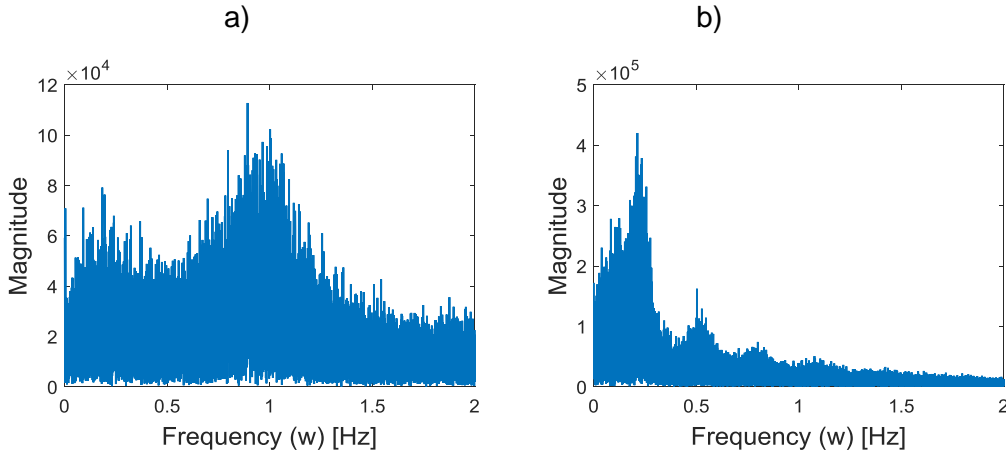


Figure 3-9: Signal of illumination in the frequency domain a) $v = 0.55$ m/s extended (0.01 Hz - 2.0 Hz). b) $v = 0.1$ m/s extended (0.01 Hz - 2.0 Hz).

Observing the spectrum of the illumination in the frequency domain, it is noticeable that the system shows several frequencies, for this case the frequencies associated with the peaks of greater height in the spectrum were taken. The illumination signal as a function of time, velocity, external illumination and time must then be represented by a series of sinusoidal oscillatory functions, with an amplitude (A_i) and a frequency (F_{pi}) and a gap (B) as shown in the equation (3-33).

$$I(v, Cb, IE, t) = \sum_{i=1}^3 A_i(v, Cb, IE) \times \sin(F_{pi}(v)t) + B(IE, Cb) \quad (3-33)$$

In this case first three main frequencies were taken, and they are shown from (3-34) to (3-39). Particles with velocities ranging from 0.05 m/s to 0.55 m/s were simulated, in figures 3-10 and 3-11 the graph for the first frequencies and the power spectrum of each frequency are shown, where a linear relationship between the variables was found.

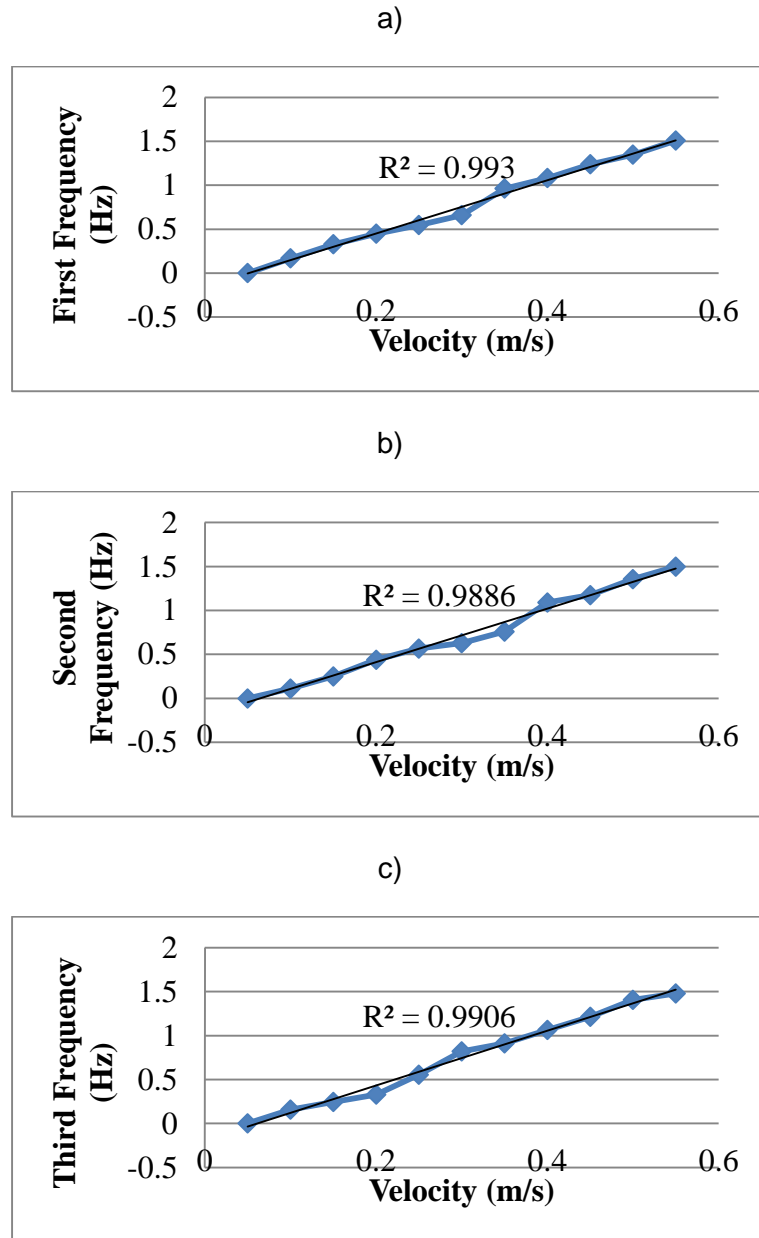


Figure 3-10: System frequencies a) first frequency b) second frequency c) third frequency.

$$F_{p1}(v) = 2.9798 \times v - 0.1362 \quad (3-34)$$

$$F_{p2}(v) = 3.0205 \times v - 0.1874 \quad (3-35)$$

$$F_{p3}(v) = 3.0546 \times v - 0.1671 \quad (3-36)$$

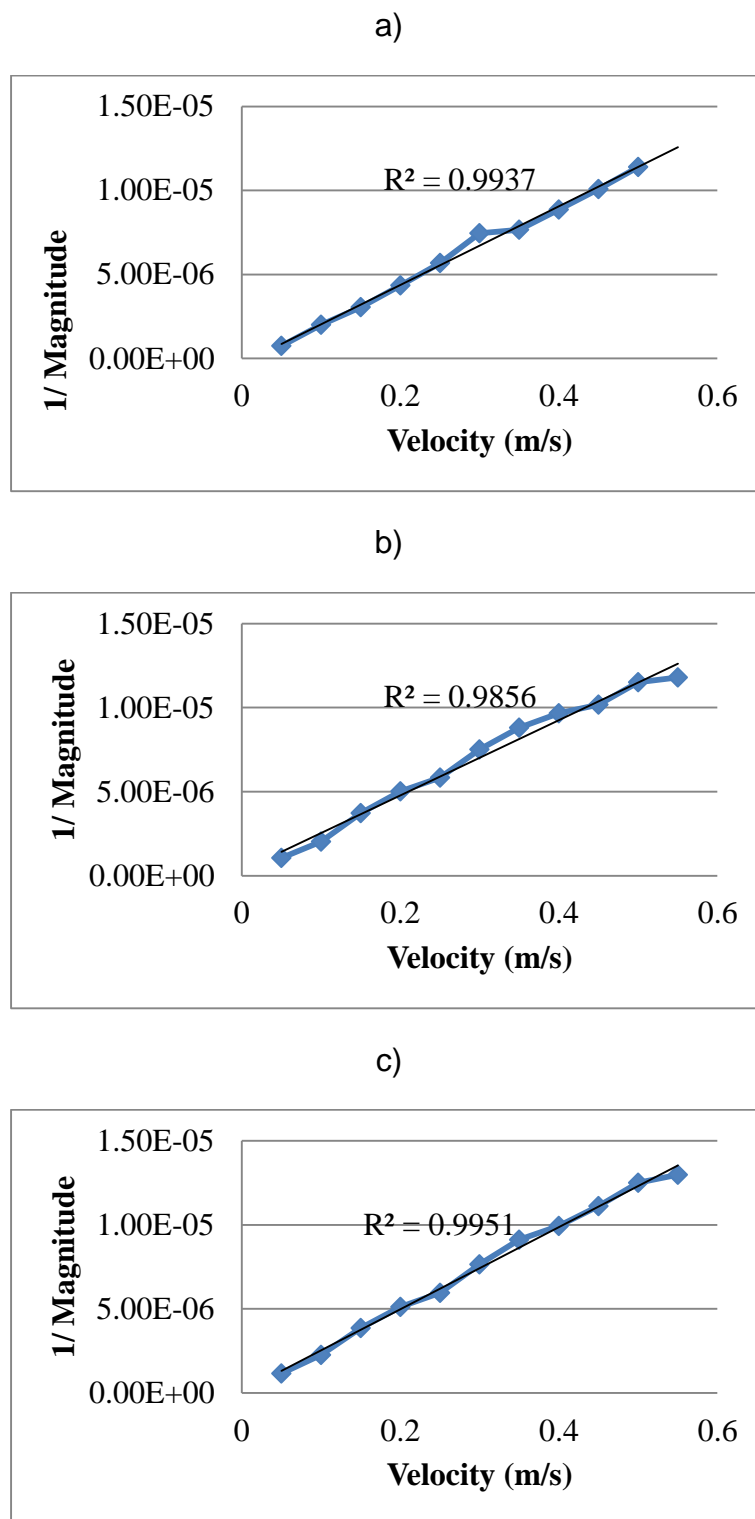


Figure 3-11: Power spectrum of the frequencies a) first frequency b) second frequency c) third frequency.

$$A_{p1}(v) = \frac{1}{2.2241 \times 10^{-5} \times v + 8 \times 10^{-8}} \quad (3-37)$$

$$A_{p2}(v) = \frac{1}{2.2241 \times 10^{-5} \times v + 2.9 \times 10^{-7}} \quad (3-38)$$

$$A_{p3}(v) = \frac{1}{2.448 \times 10^{-5} \times v + 8 \times 10^{-8}} \quad (3-39)$$

Finally, in order to take into account the variations of the illumination profile with other variables, such as: initial Biomass concentration and External illumination; it was defined the attenuation (At) variable presented in (3-40). It is a number ranging from 0 to 1, and it gives a summary of how is absorbed the light inside the PBR. The maximum illumination (I_{max}) correspond to the external illumination arriving to the surface of the reactor, the minimum illumination (I_{min}) is the illumination at the bottom of the PBR, after the capture of light over all the culture and the medium.

$$At = \frac{I_{max} - I_{min}}{I_{max}} \quad (3-40)$$

It was tested the attenuation value for biomass concentration ranging from $8.0 \times 10^2 \text{ cel/ml}$ to $8.0 \times 10^8 \text{ cel/ml}$ using 12 values, under constant external illumination of the system. Those results were shown in the Figure 3-12, with logarithmic scale, due to the wide order of magnitude of the range for biomass concentration. It was shown that with low values of the biomass concentration, the attenuation is close to zero, it means the culture does not use much energy from the illumination. On the other hand, for high values of the biomass concentration, the attenuation is close to one, it means the culture is able to use a huge amount of the energy of the illumination provided by the sun.

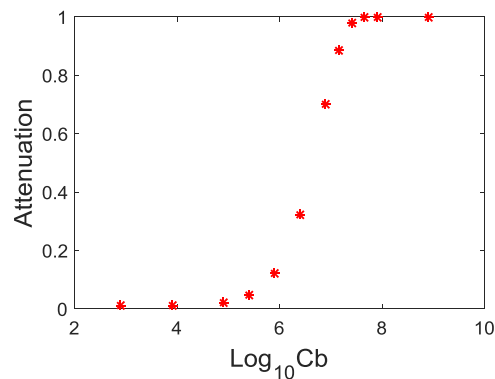


Figure 3-12: Attenuation as function of biomass concentration

In order to predict the behavior of the attenuation of the system, it was proposed to fit the data with a curve, after using some functions such as: hyperbolic functions and trigonometric functions, the best fit of the data was using an inverse tangent function, in the form showed in (3-41). The values for the parameters found are shown in Table 3-3.

$$At = B \tan^{-1}(Cx + D) + E \tag{3-41}$$

$$x = \log_{10} Cb$$

Table 3-3: Parameters of the identified function for attenuation.

Parameter	Value
<i>B</i>	0.3639
<i>C</i>	2.7627
<i>D</i>	-18.43
<i>E</i>	0.5335

The attenuation model is plotted in the figure 3-13. The proposed model for the attenuation variable achieves high prediction errors close to zero and one values, and it has to be used carefully in those regions.

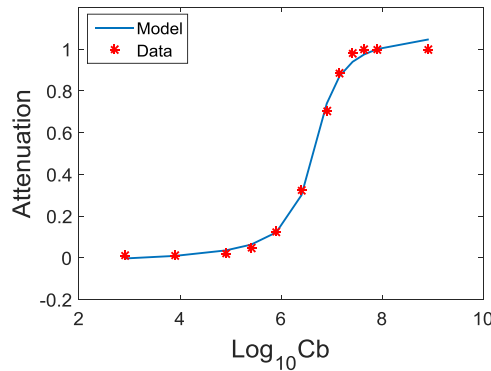


Figure 3-13: Attenuation as function of biomass concentration prediction model

The last variable involved in the illumination and LD cycles performance is the external illumination. In order to model the effect of its variations, it was tested the attenuation variable for different biomass concentrations, and also different external illuminations, ranging from $450 \mu E/m^2s$ to $1350 \mu E/m^2s$, using 3 different values. Results are shown in

figure 3-14. It is evident that external illumination does not show influence on the attenuation values.

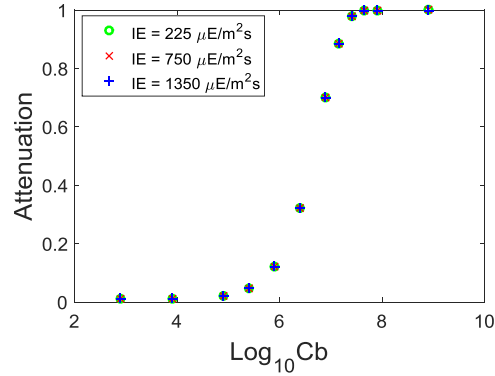


Figure 3-14: Attenuation for different external illumination and biomass concentration.

After analyzing all the results of this section, regarding to the LD frequencies, velocities, biomass concentration and external illumination it is possible to establish the illumination function in the equation (3-42), where B is calculated with (3-43) and A_i with (3-44), and the At with (3-41).

$$I(v, Cb, IE, t) = \sum_{i=1}^3 A_i(v, Cb, IE) \times \sin(F_i(v)t) + B(IE, Cb) \quad (3-42)$$

$$B(IE, Cb) = IE - At(Cb) \times \frac{IE}{2} \quad (3-43)$$

$$A_i(v, Cb, IE) = \frac{A_{pi}(v)}{2 \times \sum_{i=1}^3 A_{pi}(v)} \times At(Cb) \times IE \quad (3-44)$$

The rebuilt profile for the average behavior of the particles with medium velocity is shown in Figure 3-15 using (3-42). In this Figure the average oscillatory behavior of the particles is shown alternating between illuminated and dark zones, this illumination profile is used in the simulation of the Photosynthesis kinetics to obtain the specific rate of growth for the microalgae, and with this to predict the behavior of the biomass and the species involved in photosynthesis.

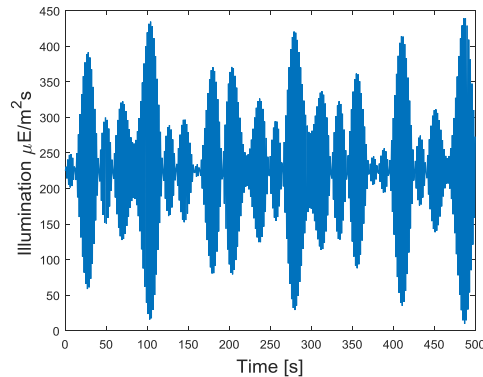


Figure 3-15: Illumination as function of time.

Figure 3-15 shows the average behavior of the illumination for the particle system in the tubular PBR, the oscillation of the received illumination between high and low values is noticeable, consequence of the trajectory generated with the static mixers in the system. The change between positions with abundant illumination and low illumination are characteristics of the LD cycles, which have been induced in the system by mixing, that is to say that the illumination profile is the function that correlates the system to the LD cycles.

In Figure 3-15 it is evident the existence of different frequencies that are related to movements that go from microalgae far from the center that gradually change to a condition close to the center. Inherently, this movement characterized by the main frequencies continue, as long as the system has enough static mixers to induce alternating particles throughout the reactor. In this sense, the mixer proposed in this project complies with carrying out an adequate mixing in the system, which contributes in a beneficial way to the LD cycles in the system, and it was correctly modelled for the PBR.

3.2 Results of dynamic model with LD cycles and PBR

This subsection presents the simulation of dynamic performance of reactants and products involved in the photosynthetic process of microalgae. Also, it is evaluated the performance of the system under disturbances.

In the table 3-4 it is shown the parameters and initial conditions used in order to simulate the performance of the PBR under constant conditions in the input of the reactor: carbon dioxide concentration ($[CO_2]_i$), oxygen concentration ($[O_2]_i$) and biomass concentration

(C_{ib}). It was used the model presented in previous sections using $n=10$, it means 10 elements analyzed for the PBR dynamics. In the Figure 3-16 it is shown the LD cycles simulation by using the illumination profile, it was built using the previously presented model.

Table 3-4: Parameters for PBR simulation

Parameter	Unit	Value
$[CO_2]_i$	mol/L	0.02
$[O_2]_i$	mol/L	0
C_{ib}	g/L	18.0151
v	m/s	0.3
IE	$\mu E/m^2s$	450

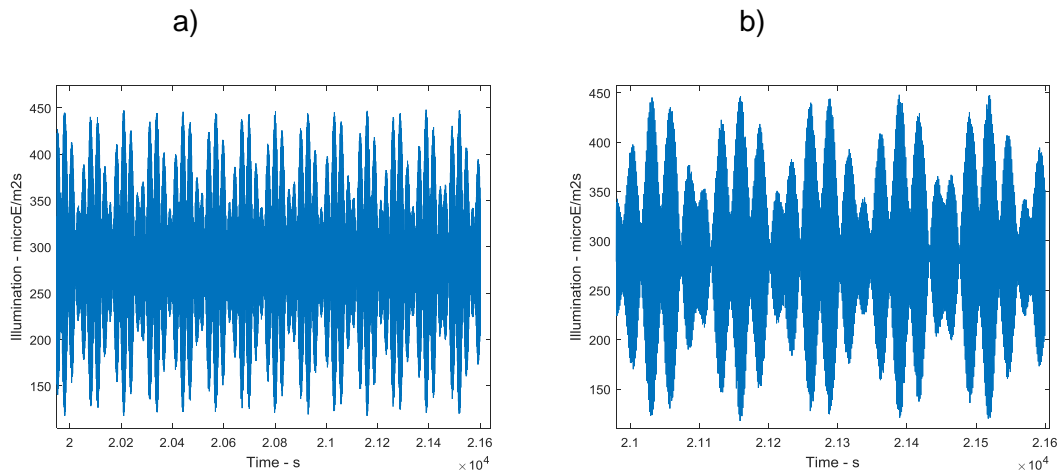


Figure 3-16: LD cycles simulation, illumination profile a) zoom 20000s – 21600 s b) zoom 21000s – 21600 s.

In the Figure 3-16, it is possible to highlight that microalgae achieve variation between illuminated and dark areas inside the PBR. According to different studies, microalgae under correct LD cycles can achieve higher productivities than those systems in which they have constant illumination. The concentration of carbon dioxide in the output of the system is shown in Figure 3-17. Initially, the concentration decreases to its minimum point, then it rises again.

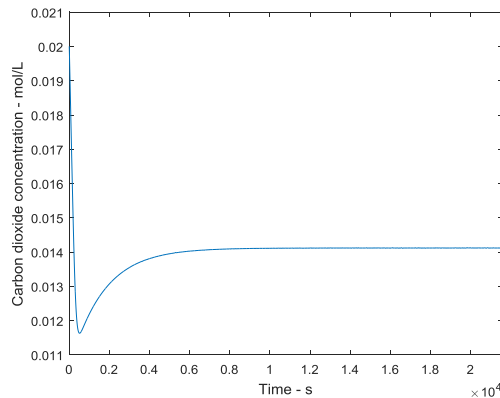


Figure 3-17: Carbon dioxide concentration output of the PBR

Oxygen and biomass concentration in the output of the system are shown in Figure 3-18 a) and b). Initially, both increase to their maximum point, after that, they descend again because of the reverse reaction to photosynthesis. In others words, the reverse reaction of photosynthetic process, in which photosynthesis is carried out, by means of the fixation of carbon dioxide and release of oxygen. The system reaches the operation point of the system after 10000 s.

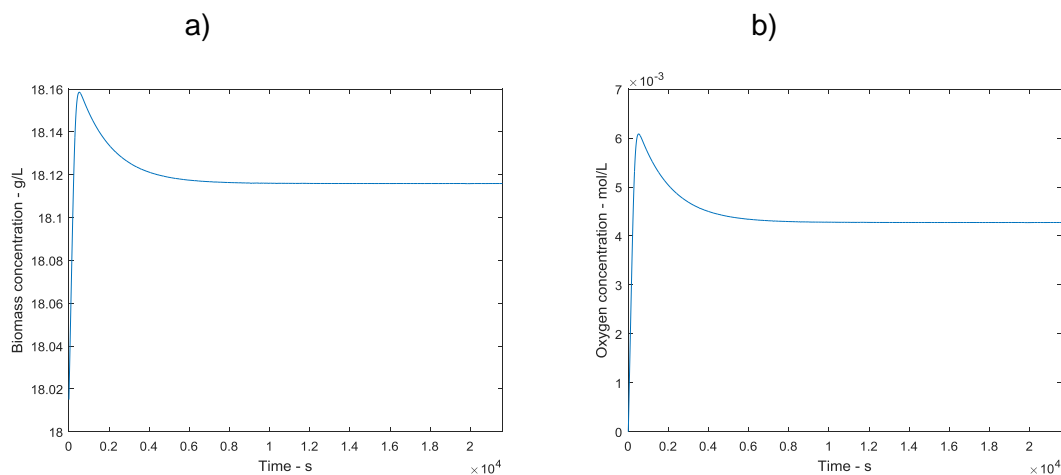


Figure 3-18: Product Dynamics a) Biomass concentration b) oxygen concentration

It is important to mention that the increase of biomass in the PBR using this model presents low values. It can be explained through the following aspects:

- This first approach of the model for the PBR is not taking into account the biomass recirculation to the system. In this model is only studied the solar receiver. For furthers

steps of this process and modelling research it is possible to expand the model to the whole PBR in order to capture biomass accumulation in all the system.

- This model is focused in fast dynamics, as the photosynthetic process in which it is appreciated the effect of LD cycles. On the contrary of the biomass, which present a slow dynamic. Photosynthesis can be done in few second, meanwhile the biomass would require several days.
- It will be required a calibration and validation experiment for this model. It will be necessary to study a specific microalgae, and to identify all the parameters and the performance coupling all the phenomena presented in this research work. It could be useful to predict in a more accurate way all the dynamic behaviors.

3.2.1 Disturbance of external illumination

External illumination is a variable important for the LD cycles prediction. The PBR can experiment variations on this variable mainly due to environment factors such as: changes on the solar hour, the total illumination received during the day has a maximum value, usually at 12h00, and has minimum values at the beginning and the end of the day. Also, presence of clouds can reduce total illumination received by microalgae inside the PBR. In the figure 3-19 it is shown a disturbance for the PBR, in which external illumination changes its value.

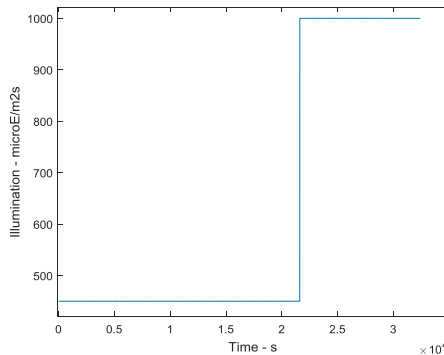


Figure 3-19: Disturbance on external illumination.

Figure 3-20 shows LD cycles prediction with a disturbance on external illumination. Mainly it affects the range between maximum and minimum value for the illumination inside the culture. So, microalgae experiment different range illumination under disturbance for the external illumination.

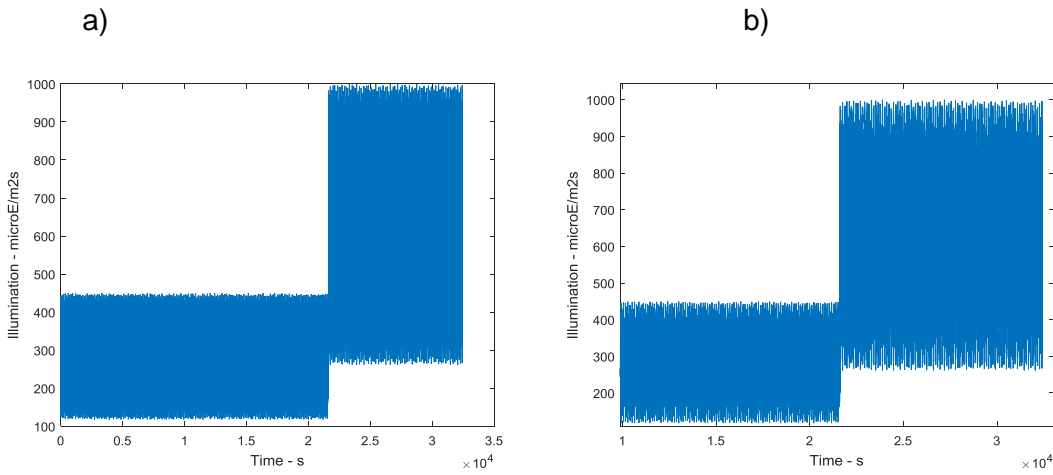


Figure 3-20: LD cycles prediction a) 0s – 32400 s b) zoom 10000s – 32400 s

In Figure 3 -21, it is shown biomass concentration in the output of the system. It increases to a maximum point, and then, it descends again due to the reverse reaction to photosynthesis. The operation point under the disturbance of external illumination is lower than the previously presented for the system under constant conditions. It means an increase of illumination received by microalgae; it can decrease the biomass concentration at the output of the reactor.

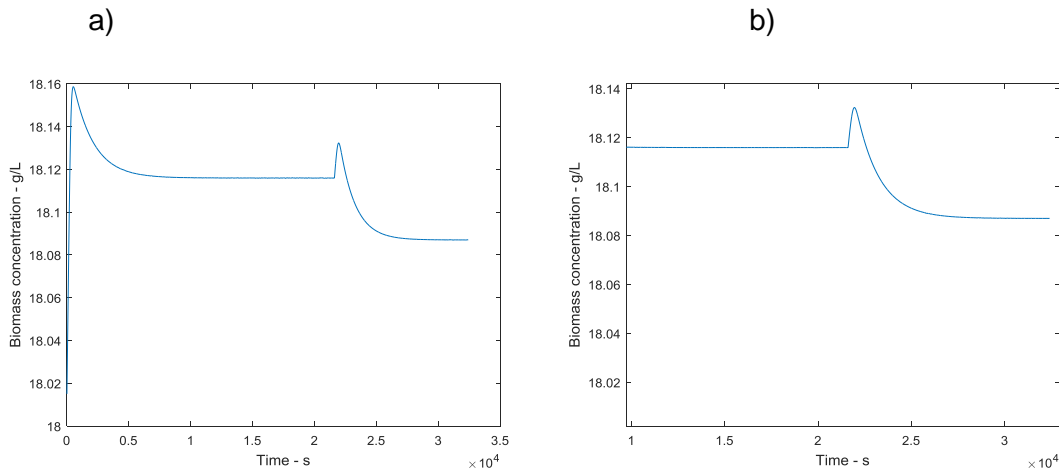


Figure 3-21: Biomass concentration output of the reactor a) 0s – 32400 s b) zoom 10000s – 32400 s

Figure 3-22 shows oxygen concentration in the output of the system. It has the same behavior of the biomass concentration. The value of the new steady state point is lower than the previously presented for constant conditions.

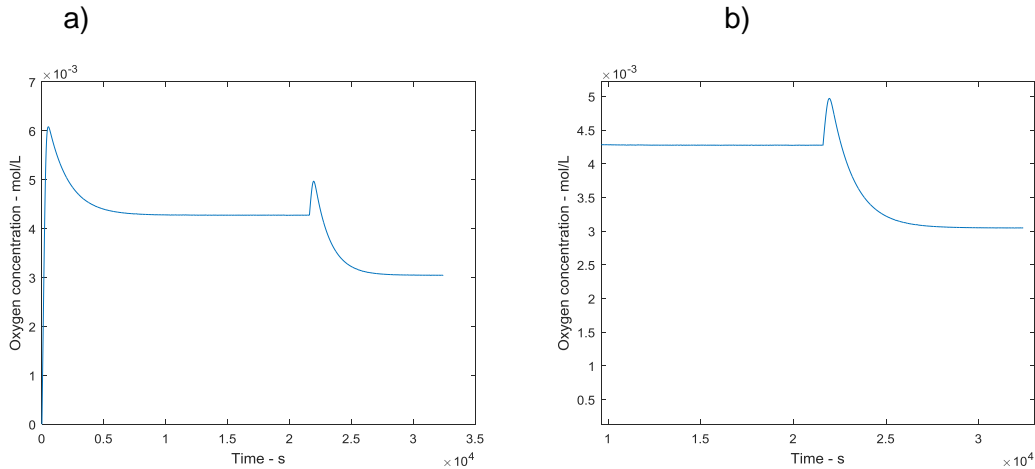


Figure 3-22: Oxygen concentration output of the reactor a) 0s – 32400 s b) zoom 10000s – 32400 s

Carbon dioxide concentration in the output of the system is shown in Figure 3-23. It decreases to a minimum point, and then it ascends again due to the reverse reaction to photosynthesis. The operation point under the disturbance of external illumination is higher than the previously achieved for the system under constant conditions.

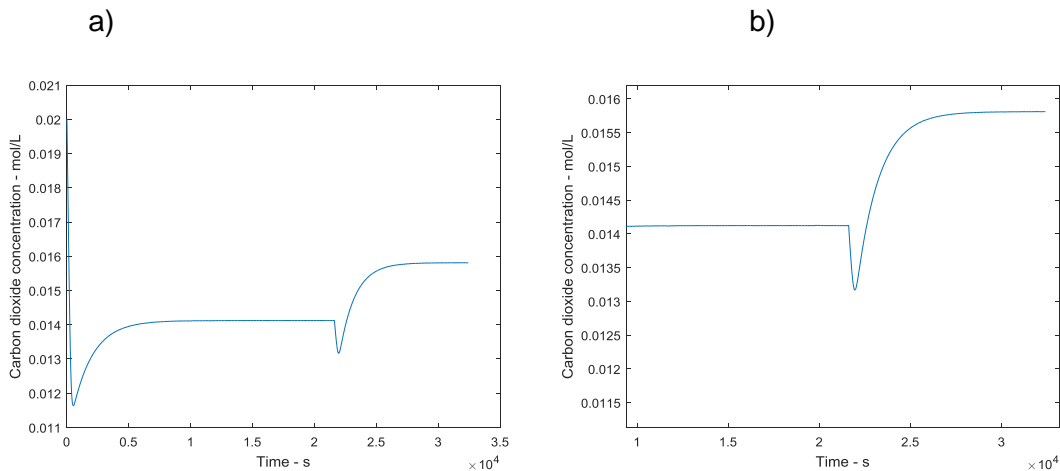


Figure 3-23: Carbon dioxide concentration output of the reactor a) 0s – 32400 s b) zoom 10000s – 32400 s

3.2.2 Disturbance of biomass concentration in the input of PBR

Initial biomass concentration in the input of the system is a variable directly related with the final biomass concentration. Due to it, it has great effect on the PBR performance. The PBR can experiment variations on this variable when there are changes of the dilution rate, and changes in the composition of culture medium. In the Figure 3-24 it is shown the disturbance for this variable.

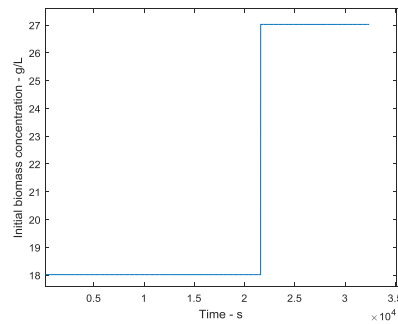


Figure 3-24: Initial biomass concentration disturbance.

Illumination received by microalgae and LD cycles are presented in the Figure 3-25. In this figure it is possible to note that variations for initial biomass concentration produce variations in the minimum value of illumination inside the reactor, it is mainly due to the fact that attenuation inside the reactor depends of both, culture medium and also biomass concentration.

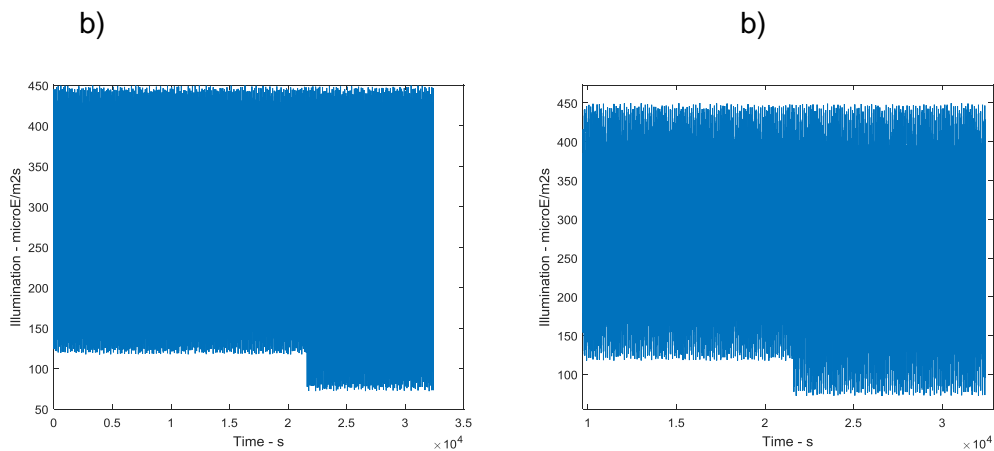


Figure 3-25: LD cycles prediction, illumination inside the culture a) 0s – 32400 s b) zoom 10000s – 32400 s

Biomass concentration in the output of the PBR is shown in Figure 3-26. As biomass concentration in the output is a variable directly related with the initial biomass concentration in the input, it has great effect. Biomass concentration in the output of the PBR increases to values similar to those of the disturbance.

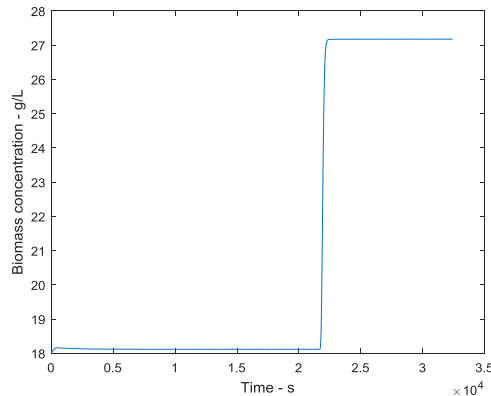


Figure 3-26: Biomass concentration in the output of the PBR 0s – 32400 s.

Oxygen concentration in the output of the reactor is shown in Figure 3-27. It increases its value and it reaches a new steady state point higher than the previously achieved under constant conditions. It is mainly due to the fact that inside the PBR there is more biomass reacting in the photosynthetic process, and so, there is more oxygen produced.

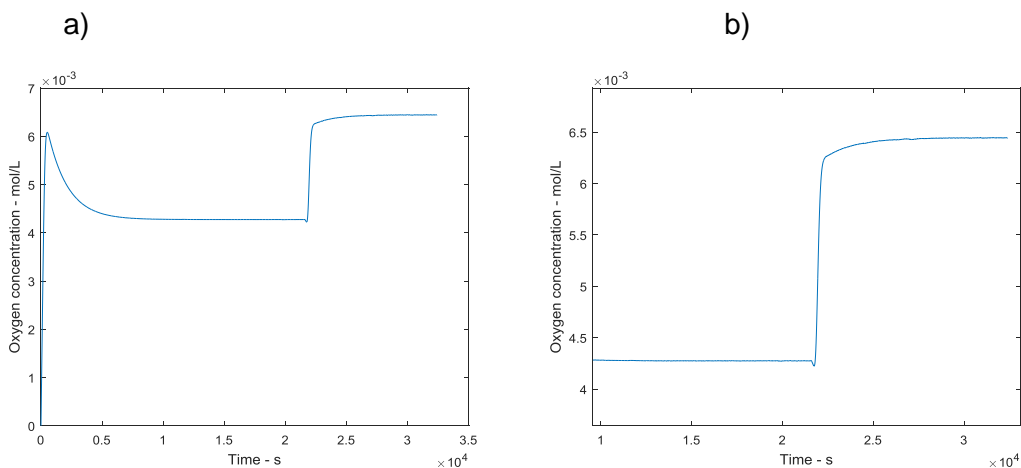


Figure 3-27: Oxygen concentration in the output of the PBR a) 0s – 32400 s b) zoom 10000s – 32400 s

Figure 3-28 shows the carbon dioxide concentration in the output of the PBR, the behavior is the opposite of the oxygen. The CO_2 concentration descends and reaches its operation

point with lower value than the previous case. This decreasing is mainly produced because the biomass inside the system has increased, and due to it, also the uptake of carbon dioxide for the photosynthetic process.

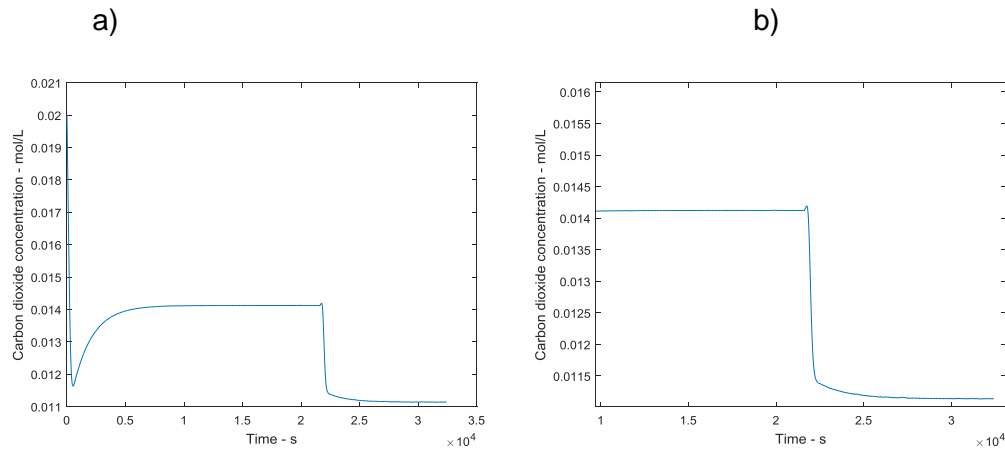


Figure 3-28: Oxygen concentration in the output of the PBR a) 0s – 32400 s b) zoom 10000s – 32400 s

3.2.3 Disturbance of velocity

As it was demonstrated in previous sections, agitation, mixing, and velocity are strongly related with the LD cycles. The main frequencies for PBR system have shown direct dependency with the velocity. The PBR can experiment variations of velocity due to agitation and mixing effects achieved by the pumping inside the PBR. In the Figure 3-29, it is shown the disturbance of velocity inside the PBR.

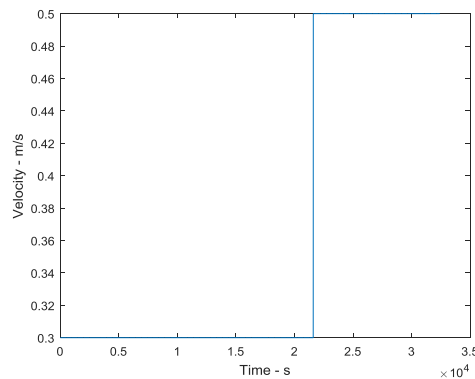


Figure 3-29: Disturbance of velocity for the system

Figure 3-30 shows Illumination received by microalgae inside the PBR. In this case, variations in velocity produce changes in the main frequencies, meanwhile the range of illumination remains constant. According to some studies productivity inside PBRs is strongly related to the frequency of LD cycles, with variations in the velocity is an easy way to have control over the LD cycles frequency, and so improving the performance of the PBR.

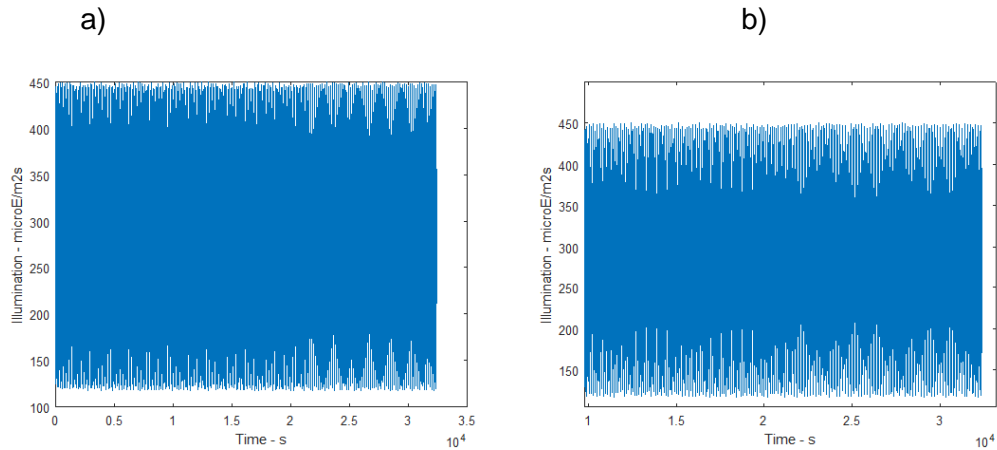


Figure 3-30: Illumination profile and LD cycles a) 0s – 32400 s b) zoom 10000s – 32400 s

Biomass concentration is shown in Figure 3-31. It decreases its value and reaches a new steady state point, with lower values than those for the previous simulation under constant conditions.

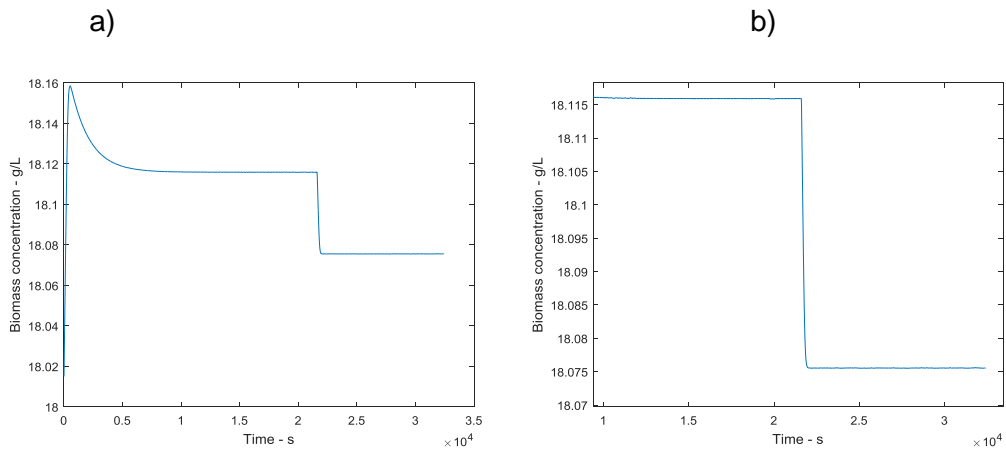


Figure 3-31: Biomass concentration in the output of the PBR a) 0s – 32400 s b) zoom 10000s – 32400 s

Oxygen concentration is shown in figure 3-32. It has similar performance to the biomass concentration.

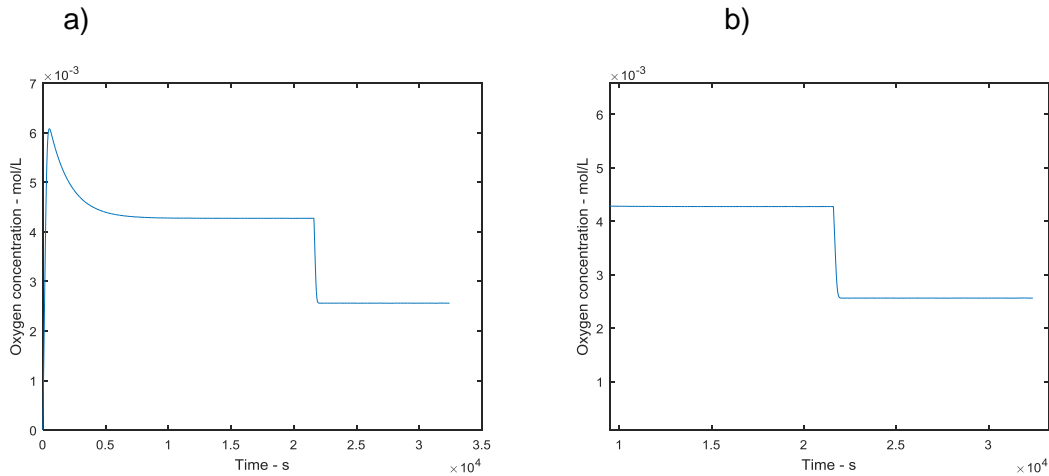


Figure 3-32: Oxygen concentration in the output of the PBR a) 0s – 32400 s b) zoom 10000s – 32400 s

Carbon dioxide concentration is shown in Figure 3-33. The concentration in the output of the reactor increases and reaches its operation point with values higher than those presented in the previous simulation.

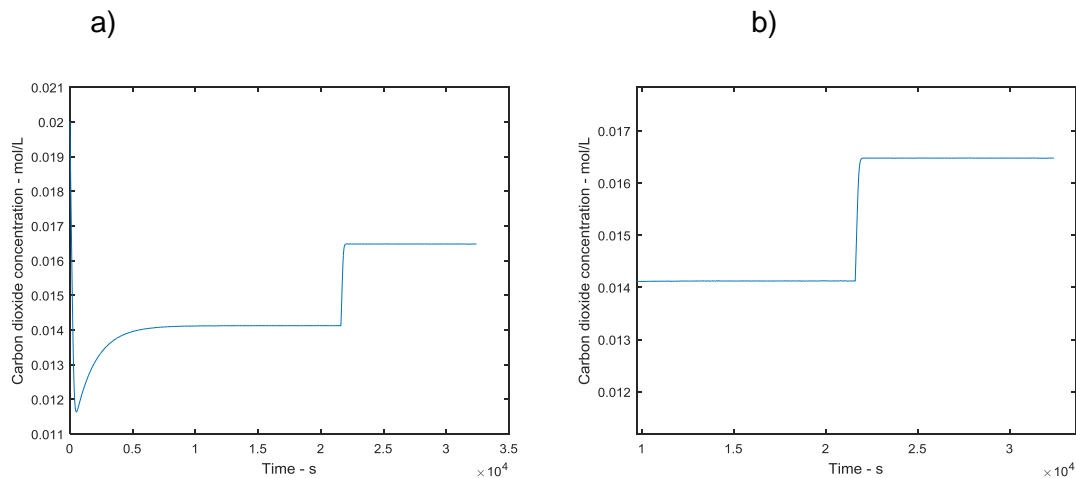


Figure 3-33: Carbon dioxide concentration in the output of the PBR a) 0s – 32400 s b) zoom 10000s – 32400 s.

According to different studies variables such as LD cycles, agitation, mixing can have significant effects on productivity of microalgae culture. This model for control purposes includes the effect of those variables on the productivity of the system. The next step then, is to evaluate some control strategies for this system in the following chapter.

3.2.4 Comparison of some variables of the PBR model with the literature

As it was showed previously, this model is not calibrated or validated. It will be required a calibration and validation experiment for this model. It will be necessary to study a specific microalgae, and to identify all the parameters and the performance coupling all the phenomena presented in this research work: hydrodynamic performance, illumination model, kinetics of photosynthesis and also the microalgae culture in PBR. It could be useful to predict in a more accurate way all the dynamic behaviors.

In this subsection it is presented a comparison of two main variables of this model. Those are the most representative variables, which make different this model from other in the literature. Those are related with the LD cycles and its effect. First variable is the frequencies of LD cycles achieved in PBR. The second variable is the specific growth rate (μ), which is affected with the LD cycles.

Table 3-5 summarizes values achieved for LD cycles frequency in other PBR studies. Normally, frequencies of LD cycles range from 0.1 Hz to 1 Hz for most of the studies presented. Some values are higher than 4 Hz, under specific conditions as shown by Gomez-Perez et al. (Gómez-Pérez, Espinosa Oviedo, Montenegro Ruiz, & van Boxtel, 2017) and the review presented by Gutierrez-Wing and colleagues (Gutierrez-Wing, Silaban, Barnett, & Rusch, 2014). Values of frequencies in this thesis are between 0.01 Hz and 1 Hz, showing similar values to those reports. It is important to highlight that the optimum LD cycles frequency is a specific variable of each microalgae, due to it, every experiment and microalgae cultivation should have different optimum values.

Table 3-5: Comparison of frequencies of LD cycles.

Frequency (Hz)	Reference	Type of study
0.2 – 0.5	Huang et al. (Huang et al., 2014).	Simulation and experimental work.
0.14	Soman et al. (Soman & Shastri, 2015).	Simulation and optimization.
0.5 – 5000	Gutierrez-Wing et al. (Gutierrez-Wing et al., 2014).	Review.
1 – 4	Gomez-Perez et al. (Gómez-Pérez et al., 2017).	Simulation.
0.1 – 1	Takache et al. (Takache, Pruvost, & Marec, 2015).	Experimental study.
0.01 – 1.5	This thesis.	Modelling

Table 3-6: Comparison of specific growth rate of PBR.

μ (h ⁻¹)	Reference	Type of study
0.024	Huang et al. (Huang et al., 2014).	Simulation and experimental work.
0.05	Soman et al. (Soman & Shastri, 2015).	Simulation and optimization.
2 – 3.	Gutierrez-Wing et al. (Gutierrez-Wing et al., 2014).	Review.
2	This thesis.	Modelling

Table 3-6 shows some values of specific growth rate. The values typically showed for those studies are lower than 3 h⁻¹. In the case of the model proposed in the thesis, the value is close to 2 h⁻¹ showing concordant values with other studies.

Chapter 4: Photobioreactor control strategies

Chapter 2 and Chapter 3 showed the proposed static mixer and the proposed PBR model in this thesis. Along this thesis and the literature review it has been shown that there are some variables which can have a huge impact in the productivity and so in the economy of the PBR process. The static mixer and the model proposed in this thesis were built taking into account some of those important variables such as: agitation and LD cycles. After that, the next step is to evaluate some control strategies which can manage the energy consumption in order to improve the performance of the PBR process under some disturbances conditions.

In this chapter, it is proposed a new energetic function, which takes into account the biomass productivity and also the energy consumption of the pumping system. It is evaluated if an EMPC strategy taking into account the energetic consumption can lead to improvements in the economy of the process. Due to the fact that PBR is a multivariable and complex system, it will be tested MPC and EMPC, which are control strategies adequate for those systems in which are involved several variables and constraints for its operation.

This chapter is organized as follows:

- Firstly, it is presented both strategies MPC and EMPC applied to PBRs. It is shown their optimization problems and constraints. Besides of that, it is presented a new energetic function, which takes into account productivity of the system, and energy consumption.
- Finally, it is presented the results of the simulation of control strategies. It is shown the reference tracking of the MPC. After that, it is compared the results for both controllers under two disturbance scenarios.

4.1 Model predictive control and economic model predictive control in photobioreactors

In this subsection it is presented the MPC and EMPC control strategies applied to tubular PBR, their objective function, constraints and optimization problem. Along with that, it is presented an energetic function proposed in this thesis, it is used for the EMPC formulation.

4.1.1 Model predictive control - MPC

The control objective was to maintain the photosynthetic efficiency at a desired level, it can be achieved by means of keeping the products concentration at a fixed level, those can be biomass or oxygen concentration. Therefore, the variable to be controlled is the oxygen concentration ($y = [O_2]$) in the output of the reactor, while the manipulated variable is the velocity ($u = v$) in the system, it has a direct relationship with the frequencies of the LD cycles, and so on with the productivity of the system.

Figure 4-1 shows a scheme of the MPC controller. Outputs of the system are related with the concentration of species at the last element analyzed of the reactor, those are: biomass concentration (C_{fb}), oxygen concentration ($[O_2]$) and carbon dioxide concentration ($[CO_2]$). Where biomass and oxygen are products in the photosynthetic process, due to it, we choose as controlled variable one of the products. The MPC controller periodically receives information from the system, in order to solve the optimization problem, which calculates an optimized value for the manipulated variable (v) periodically.

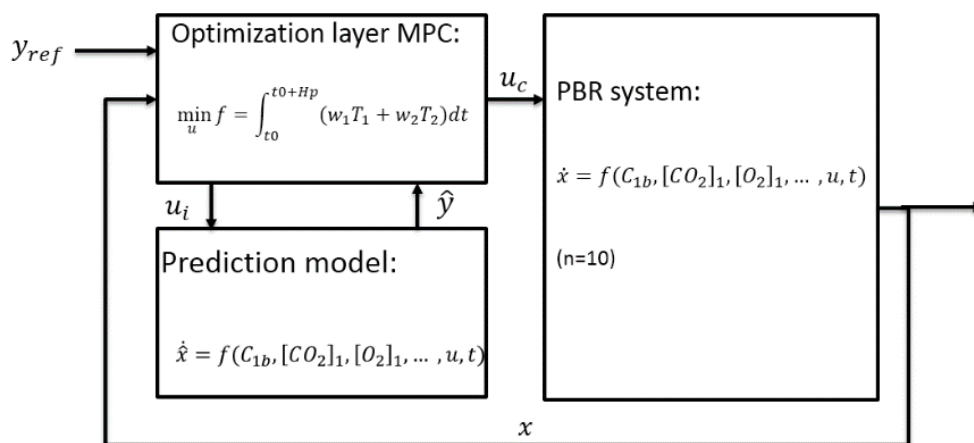


Figure 4-1: Control scheme MPC

The objective function is presented in (4-1), it has two main terms related to the regulation problem, and also the variations for the control action, in this case the velocity. The objective function was evaluated by means of the integral during the prediction horizon (H_p).

$$\min_u f = \int_{t_0}^{t_0+H_p} (w_1 T_1 + w_2 T_2) dt \quad (4-1)$$

The first term presented in (4-2), is the regulatory problem, in which it is pretended that the controller reaches the reference value, obtained from an offline optimization. The second term (4-3) has the function to regulate that variations of control actions between one step and the next one are low, it avoids sudden changes on the actuator of the system. It helps to find the best trajectory, and with the lowest variations among the subsequent steps.

$$T_1 = (y - y_{ref})^2 \quad (4-2)$$

$$T_2 = (u_i - u_{i-1})^2 \quad (4-3)$$

As it was shown previously, after the system is under disturbances of velocity (chosen as manipulated variable) the system can take a minimum time of 400 s reaching the new steady state point. Due to that, prediction horizon (H_p) was fixed in a higher value as it is 500 s. It was chosen an MPC problem with three steps of control with a total control horizon of 300 s, time less than the prediction horizon. Weights (w_1 and w_2) were chosen in order to give more importance to the regulatory term. Reference was calculated using a static offline optimization of the function presented in the next subsection related to the Energetic function.

Prediction horizon was 500 s according to the dynamics of the model presented in this thesis and also the results of the model under disturbances. A control horizon (H_c) of 300 s. The time elapsed between two consecutive controls actions was 100 s. The weights for the first and second term were 0.7 and 0.3 respectively. The reference was 0.005 mol/L. Once all those values are fixed, the optimization problem is defined, they are presented from (4-5) to (4-7).

$$H_p = 500 \text{ s} \quad H_c = 300 \text{ s} \quad (4-4)$$

$$\Delta t_u = 100 \text{ s} \quad (4-5)$$

$$y_{ref} = \frac{0.0055 \text{ mol}}{L} \quad (4-6)$$

$$w_1 = 0.7 \quad w_2 = 0.3 \quad (4-7)$$

The operation of a PBR has associated diverse constraints, which are given by installed capacities, values in the concentration of biomass and chemical species, intervals for the variables and the principles of conservation of mass and momentum involved in the models.

The MPC optimization problem has the following constraints:

- All variables must be non-negative, due to the fact that the system is the photosynthetic production, and all species involved are present.
- Velocity can take values from 0.05 m/s to 0.55 m/s. Due to the fact that initially this model has been tested between those values.

$$u_i \in (0.05, 0.55) \quad (4-8)$$

- The photosynthetic process has associated the equations of the growth kinetics and LD cycles presented previously in the Chapter 3. Those can be summarized in the expression (4-9)

$$h(\dot{x}_1, \dot{x}_2, \dot{x}_3, x_1, x_2, x_3, I, \mu) = 0 \quad (4-9)$$

- Finally, the system must comply the PBR model presented in the Chapter 3, this can be represented in an abbreviated way in the expression (4-10).

$$g([\dot{CO}_2], [O_2], \dot{c}_b, [CO_2], [O_2], c_b) = 0 \quad (4-10)$$

The optimization problem presented in this section can be summarized as follows:

$$\min_u f = \int_{t_0}^{t_0+Hp} (w_1 T_1 + w_2 T_2) dt \quad (4-1)$$

Subject to:

$$h(\dot{x}_1, \dot{x}_2, \dot{x}_3, x_1, x_2, x_3, I, \mu) = 0 \quad (4-9)$$

$$g([\dot{CO}_2], [O_2], \dot{c}_b, [CO_2], [O_2], c_b) = 0 \quad (4-10)$$

$$u_i \in (0.05, 0.55) \quad (4-8)$$

Where h represents the constraints related to the kinetic model and g represent the model of the PBR.

4.1.2 Energetic function

The aim of this thesis is to evaluate if it is possible to improve the economy of the tubular PBR. Due to it, the static mixer presented in Chapter 2 and the PBR model proposed presented in Chapter 3 on this thesis are focused in variables such as: agitation, mixing and the effect of LD cycles. Those variables are strongly related with the productivity and the energy consumption for this system. As it was previously showed agitation and mixing represent values close to 70% (N. H. Norsker, Barbosa, Vermuë, & Wijffels, 2011) of all energy consumption.

The profitability, or economic benefit, of the photosynthetic process carried out in the PBR is reflected in variables such as: energy consumption of the system, and the produced energy of the system. Therefore, it is proposed an optimization in terms of energy for the system, in that way, also it is possible to avoid huge variations in prices, depending on the final application of the biomass. It is intended to evaluate how much energy the PBR consumes in its operation, and how much energy is produced by the microalgae.

In this thesis, we propose a function that calculates the amount of net energy in the system, showed in (4-11). It is assumed that microalgae can generate an amount of energy equivalent to its combustion heat, it means we assumed that microalgae can carry out a complete combustion. The majority of energy consumed by the tubular PBR is associated with the pumping of the culture, as it was shown in 2011 by Norsker (N.-H. Norsker et al., 2011). Therefore, it is considered only the effect of energy consumption associated with the operation of the pumping system, this energy consumption is taken into account as the kinetic energy supply to the fluid.

$$E_{net} = E_{biom} - E_{pump} \quad (4-11)$$

The energy that can be obtained with the biomass produced in the reactor is related to the combustion heat according to (4-12).

$$E_{biom} = v_b A (C_{fb} - C_{ib}) \Delta H_b \quad (4-12)$$

Where A is the cross-sectional area, v_b is the average flow velocity, C_{fb} and C_{ib} are the concentration of biomass at the output and input of the tubular section of the PBR respectively. Finally ΔH_b is the combustion heat of the microalgae, referred to values close to 20 KJ/g (Garcia C., 2012) according to an experimental study of several species of microalgae.

Deriving from the definition of pressure, which express a force exerted per unit of area, once it is known the cross-sectional area, it is possible to calculate an average force of the fluid. Additionally, when it is known the average flow velocity (v_b), and the average force of the fluid (N_b), it is possible to estimate the energy required for the pumping system using (4-13). Where ΔP_b is the pressure drop of the system, which is indirectly related to the pressure that pumping system must supply. Pressure drop as function of velocity is shown in Annex A.

$$E_{bomba} = N_b v_b = v_b A \frac{N_b}{A} = v_b A \Delta P_b \quad (4-13)$$

By replacing (4-13) and (4-12) in (4-11), it is then obtained an expression for net energy of the PBR. It is shown in (4-14).

$$E_{net} = v_b A (C_{fb} - C_{ib}) \Delta H_b - v_b A \Delta P_b \quad (4-14)$$

This energetic function can be used as it was shown in (4-14). Nevertheless, it can be used both terms (4-13) and (4-12) individually, in order to have different weights of the energy in case of a multiojective optimization problem, where it could be possible to give more importance to one of those terms.

4.1.3 Economic Model predictive control - EMPC

For the EMPC strategy the control objective was to maintain the economic benefit of the PBR at a maximum level, and so the net energy of the system. Net energy is directly related to the economy of the process, and with economic feasibility of those systems. Due to the above, it was taken into account for the EMPC control.

Figure 4-2 shows a scheme of the EMPC controller. Outputs of the system are related with the concentration of species at the last element analyzed of the reactor, those are: biomass concentration (C_{fb}), oxygen concentration ($[O_2]$) and carbon dioxide concentration ($[CO_2]$).

As it was shown previously, with the flow velocity and the biomass concentration it is possible to estimate the net energy of the PBR operation. The EMPC controller receives information from the system, in order to solve the optimization problem, which calculates an optimized value for the manipulated variable (v) periodically.

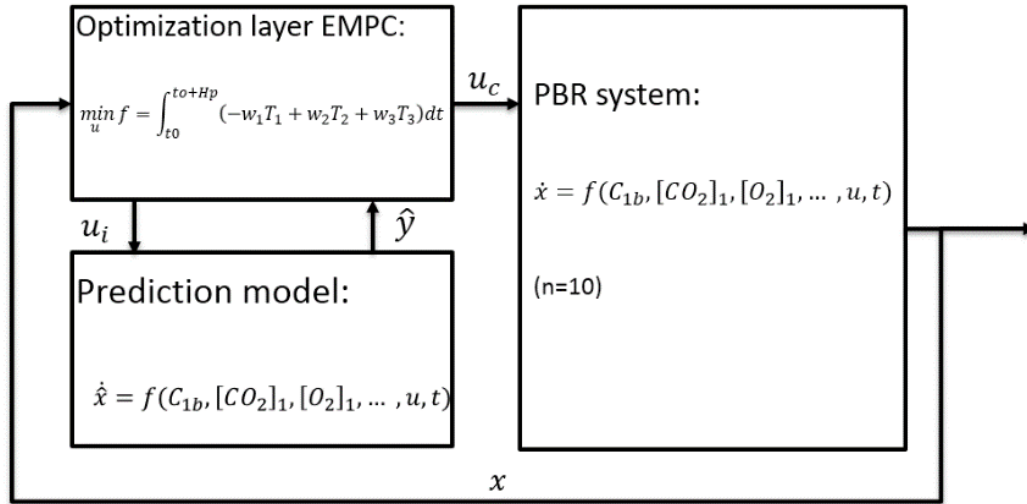


Figure 4-2: Control scheme EMPC

The objective function is presented in (4-15), it has two main terms related to the optimization of energy, the economic variable, and also the variations of the control action, in this case the velocity. The objective function was evaluated by means of the integral during the prediction horizon (H_p).

$$\min_u f = \int_{t_0}^{t_0+H_p} (-w_1 T_1 + w_2 T_2 + w_3 T_3) dt \quad (4-15)$$

The first and second term presented in (4-16), are terms related to the objective function which takes into account energetic aspects, and they were presented previously in this chapter. The negative part of this terms is the conversion of the biomass produced inside the PBR to an energetic term. The positive part of this terms is the pumping energy required by the system, in order to achieve a productivity. This objective function takes into account both actions, how much energy the PBR can produce, and also how much energy is used by the PBR for pumping purposes.

$$T_1 = u_i A (C_{fb} - C_{ib}) \Delta H_b \quad T_2 = u_i A \Delta P_b \quad (4-16)$$

The third term (4-17) has the function to regulate the variations of manipulated variable between one step and the next one. With this term the variations are low, it avoids sudden changes on the actuator of the system. It helps to follow the best trajectory, and with the lowest variations among the next steps. Those terms were added because the EMPC objective function is non-convex, and due to it, it can be unstable and arrive to local minimum solution, with this third term it is possible to offer a trajectory with the lowest changes on the manipulated variable, and so moving to the closets minimum of the optimization problem.

$$T_3 = (u_i - u_{i-1})^2 \quad (4-17)$$

As it was shown previously, after the system is under disturbances of velocity (chosen as manipulated variable) the system can take a between 400 s to 2000 s reaching the new steady state point. Due to that, prediction horizon (H_p) was fixed in a higher value as it is 2500 s. It was chosen an EMPC problem with three steps of control with a total control horizon of 1500 s, time less than the prediction horizon. Weights (w_1 , w_2 and w_3) were chosen in order to give more importance to the pumping energy, biomass energy.

Prediction horizon was 2500 s according to the dynamics of the model presented in this thesis and also the results of the model under disturbances. A control horizon (H_c) of 1500 s. The time elapsed between two consecutive controls actions was 500 s. The weights for the first, second and third term were 1, 20 and 0.3 respectively. After all those values are fixed, the optimization problem is well defined, they are presented from (4-18) to (4-20).

$$H_p = 2500 \text{ s} \quad H_c = 1500 \text{ s} \quad (4-18)$$

$$\Delta t_u = 500 \text{ s} \quad (4-19)$$

$$w_1 = 1 \quad w_2 = 20 \quad w_3 = 0.3 \quad (4-20)$$

The EMPC optimization problem has the following constraints:

- All variables must be non-negative, due to the fact that the system is the photosynthetic production, and all species involved are present.
- Velocity can take values from 0.05 m/s to 0.55 m/s. Due to the fact that initially this model has been tested between those values.

$$u_i \in (0.05, 0.55) \quad (4-21)$$

- The photosynthetic process has associated the equations of the growth kinetics and LD cycles presented previously in the Chapter 3. Those can be summarized in the expression (4-22)

$$h(\dot{x}_1, \dot{x}_2, \dot{x}_3, x_1, x_2, x_3, I, \mu) = 0 \quad (4-22)$$

- Finally, the system must comply the PBR model presented in the Chapter 3, this can be represented in an abbreviated way in the expression (4-23).

$$g([\dot{CO}_2], [O_2], \dot{C}_b, [CO_2], [O_2], C_b) = 0 \quad (4-23)$$

The optimization problem presented in this section can be summarized as follows:

$$\min_u f = \int_{t_0}^{t_0+Hp} (-w_1 T_1 + w_2 T_2 + w_3 T_3) dt \quad (4-15)$$

Subject to:

$$h(\dot{x}_1, \dot{x}_2, \dot{x}_3, x_1, x_2, x_3, I, \mu) = 0 \quad (4-22)$$

$$g([\dot{CO}_2], [O_2], \dot{C}_b, [CO_2], [O_2], C_b) = 0 \quad (4-23)$$

$$u_i \in (0.05, 0.55) \quad (4-21)$$

Where h represents the constrains related to the kinetic model and g represent the model of the PBR.

4.2 Results of the MPC and EMPC controllers

In this subsection are presented the main results for both controllers, in two scenarios that can be considered as normal for a real implementation of the PBR. The first scenario present variations of the external illumination and the second, variations of the initial biomass concentration.

4.2.1 Reference Tracking MPC

In this section it is presented the results of the MPC controller for reference tracking, it was tested two references. First reference is presented in Figure 4-3. Second reference is presented in Figure 4-4.

PBR system was simulated in open loop during 21600 s, after that, the MPC controller starts to operate. In Figure 4-3 it is shown that the MPC controller proposed in this thesis is able to reach the first reference 0.005 for the product oxygen concentration and keep the system there in few control actions, under constant conditions.

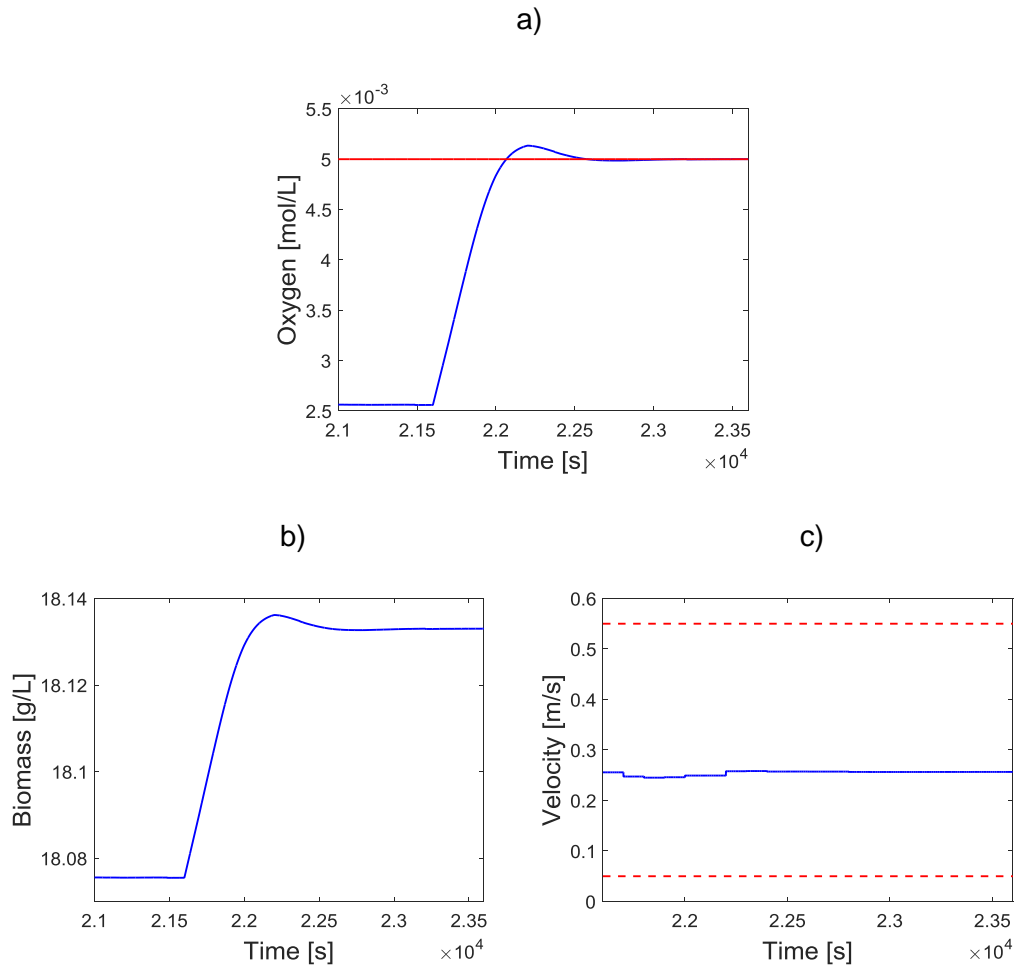


Figure 4-3: MPC reference tracking Ref = 0.005 mol/l a) Oxygen concentration b) Biomass concentration c) Velocity

PBR system was simulated in open loop during 21600 s, after that, the MPC controller begins its function. In Figure 4-4 it is shown that the MPC controller proposed in this thesis is able to reach the second reference 0.0055 for the product oxygen concentration and keep the system there in few control actions, under constant conditions.

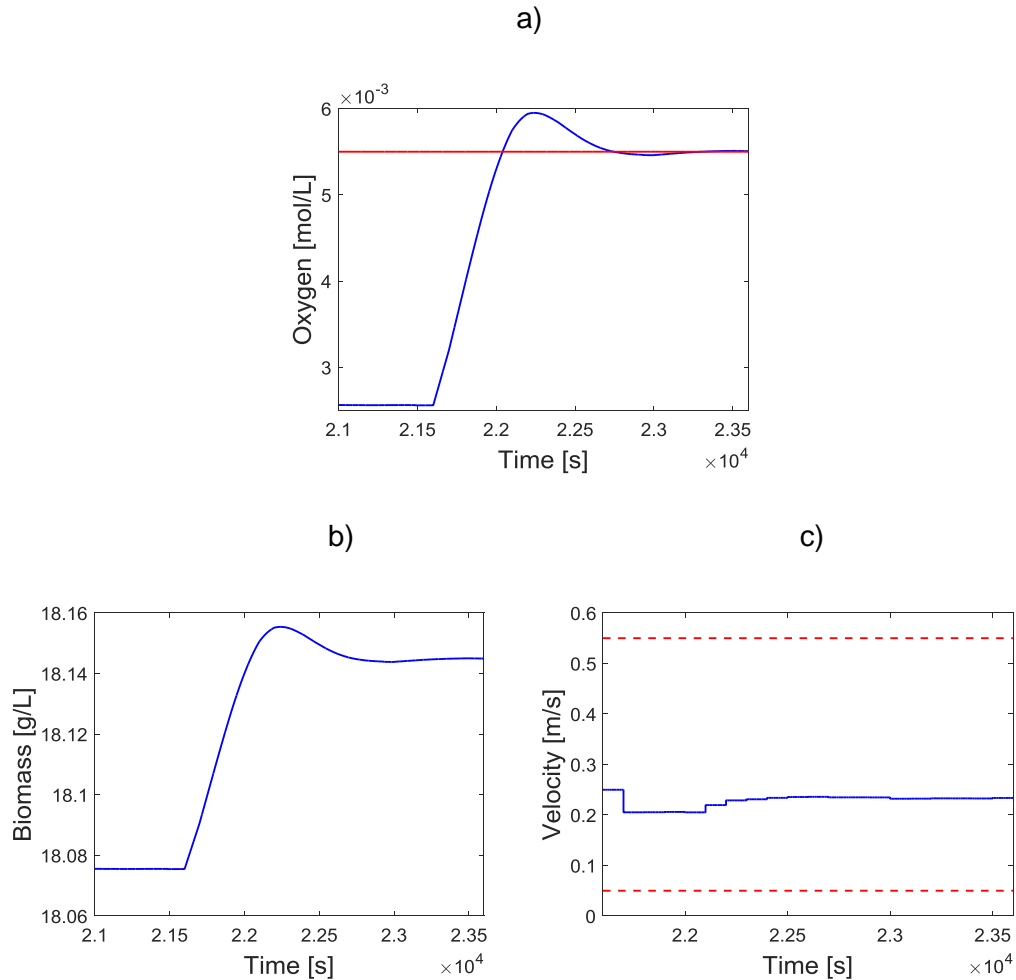


Figure 4-4: MPC reference tracking Ref = 0.0055 mol/l a) Oxygen concentration b) Biomass concentration c) Velocity

4.2.2 Scenario 1

The first scenario takes into account variations for the external illumination, it means the illumination available for the photosynthetic process. During the daily operation inside the PBR, illumination at the beginning of the day has low values, it increases achieving a maximum value at 12h00, and then it decreases all of this considering an ideal scenario. So, the lowest values for illumination are presented at the beginning and at the end of the day. Figure 4-5 a) shows the illumination profile during the day and Figure 4-5 b) shows the biomass concentration in the system under a normal day operation. It is noticed that high

values of the external illumination at noon, reduce the productivity of the system, mainly due to the photoinhibition in which microalgae receive more energy than they need, and because of that, they are damaged.

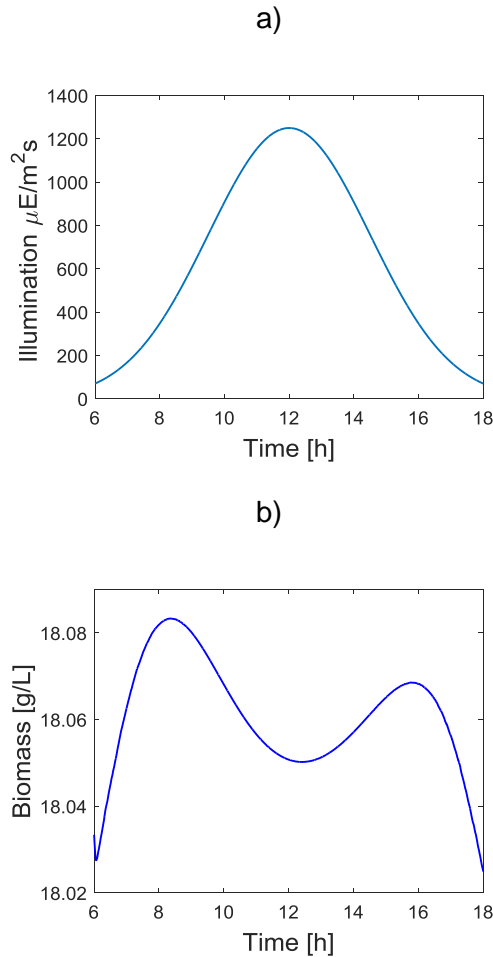


Figure 4-5: Day operation profile a) Illumination b) biomass concentration.

Figure 4-6 shows the results of MPC controller. In this figure it is possible to note that the system reaches values close to the reference, but with some oscillations around the reference value. Taking into account that the MPC controller under constant conditions is able to reach reference values, once the perturbation is always affecting the system, like the case of the external illumination, the proposed MPC is close to the reference most of the time, but not exactly in the reference value.

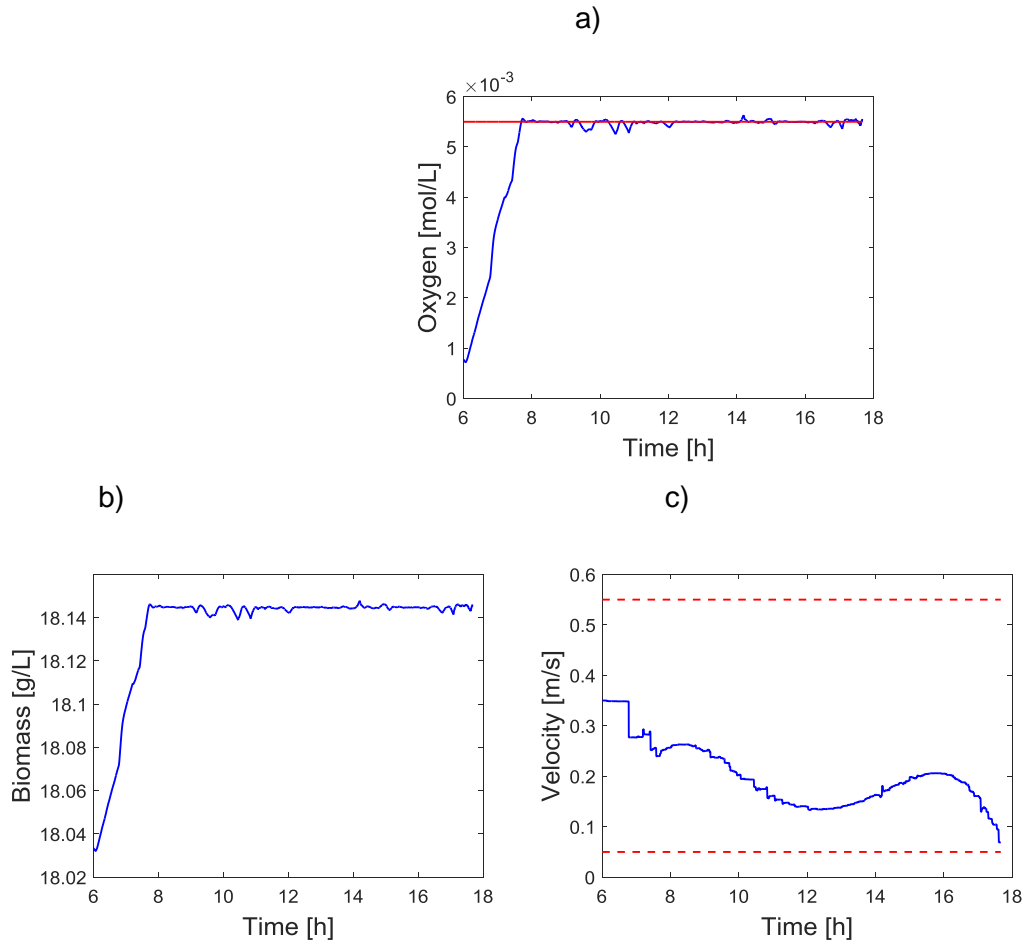


Figure 4-6: MPC results for scenario 1 a) Oxygen concentration b) Biomass concentration c) Velocity

Also it is noticeable that in the Figure 4-5 a) there are basically two regions for the disturbance, first half of the day illumination increases its values, and the second half of the day it decreases. Nevertheless, the system in Figure 4-5 b) present four regions, due to the effect of illumination and photoinhibition inside the microalgae culture, those are:

- First region, productivity of the system increases to its maximum value.
- Second region, productivity decreases to its minimum value.
- Third region, productivity increases.
- Finally, productivity decreases.

MPC controller present some values far from the reference close to the points of transition between one region and the next one, mainly because MPC receives information of the

states of the system, but it is not able to predict future effects of the disturbances. Figure 4-7 shows the EMPC results for scenario 1 and Figure 4-8 presents the comparison of MPC controller, EMPC controller and the open loop. The EMPC controller can reach higher values than the MPC controller, in some regions. Nevertheless, the EMPC controller uses as objective function the energetic function presented previously, which is a non-convex function. Due to it, the EMPC optimization problem can present problems of to be unstable or to reach local minima. It is noticeable that in some regions, EMPC controller is able to reach higher values than the reference value of the MPC, which was obtained from a static optimization layer. It means, that for the PBR under illumination disturbances a reference value obtained from a static optimization may not be adequate.

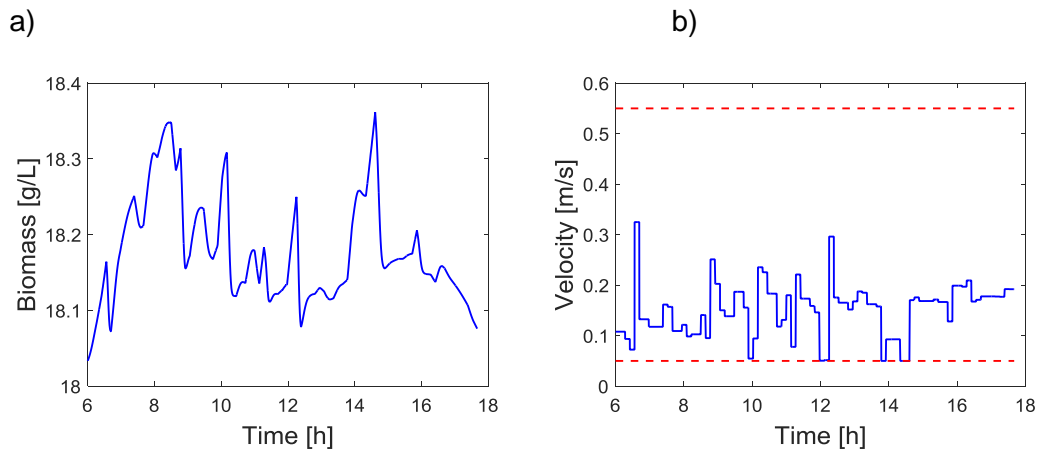


Figure 4-7: EMPC results for scenario 1 a) biomass concentration b) velocity

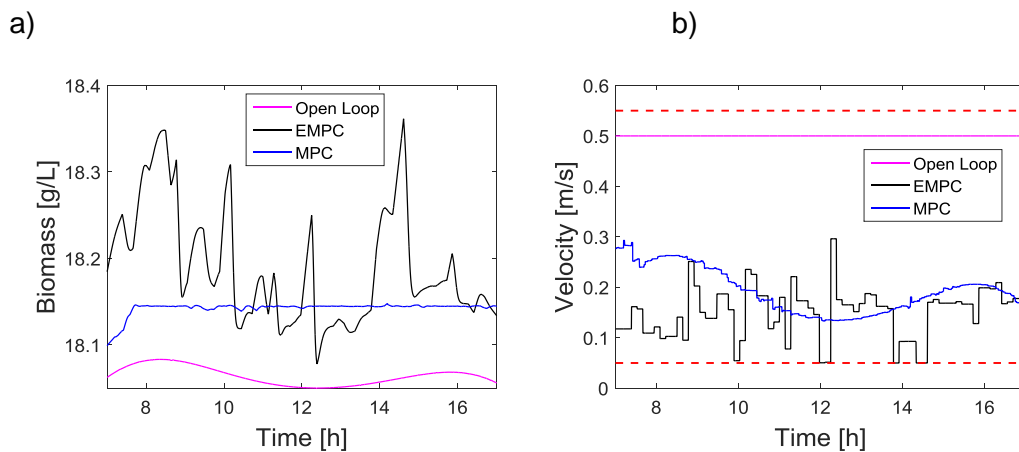


Figure 4-8: Comparison of results for scenario 1 a) biomass concentration b) velocity

In this thesis, it was proposed the energetic function, and both terms: first related to the biomass energy and pumping energy. This function was proposed mainly to the fact that biomass prices have a wide range from 400 €/ton to 900000 €/ton, depending of the final application and post-processing costs (Barsanti & Gualtieri, 2018). For further studies, and a fixed application it can be proposed an economic function which takes into account prices of biomass. In order to make priority the energetic savings for the PBR system, it was assigned a high value of weight ($w_2 = 20$) to the pumping energy. In that way, the EMPC controller is able to manage the system in order to produce a good amount of biomass, and at the same time saving energy as much as possible.

EMPC controller showed high dependency to the tuning parameters such as: weights and prediction and control horizons. The results obtained in this thesis are good, but they could be better by means of performing an optimization of the parameters of the controllers. Other improvement of EMPC controller would be to study other ways of the multi-objective optimization.

4.2.3 Scenario 2

The second scenario takes into account variations of the initial biomass concentration, under constant illumination condition. The variations of the initial biomass can have diverse origins such as:

- Damages of the pumping system, in that case, biomass concentration could present variations.
- Increments and decrements of the dilution rate for the PBR.
- Variation in the composition of the culture medium.

Due to the possibility of those variations it was simulated the second scenario, in which it is presented increments and decrements of the initial biomass concentration. It is shown in the Figure 4-9 a) and b). The PBR under disturbance of the biomass concentration shows a trajectory similar to the disturbance. This is mainly to the fact that biomass concentration in the output of the reactor is directly related with the initial biomass concentration in the input of the same. Besides of that, the biomass variation between input and output is not very big, due to it, it is not able to mitigate at all the disturbance affectation.

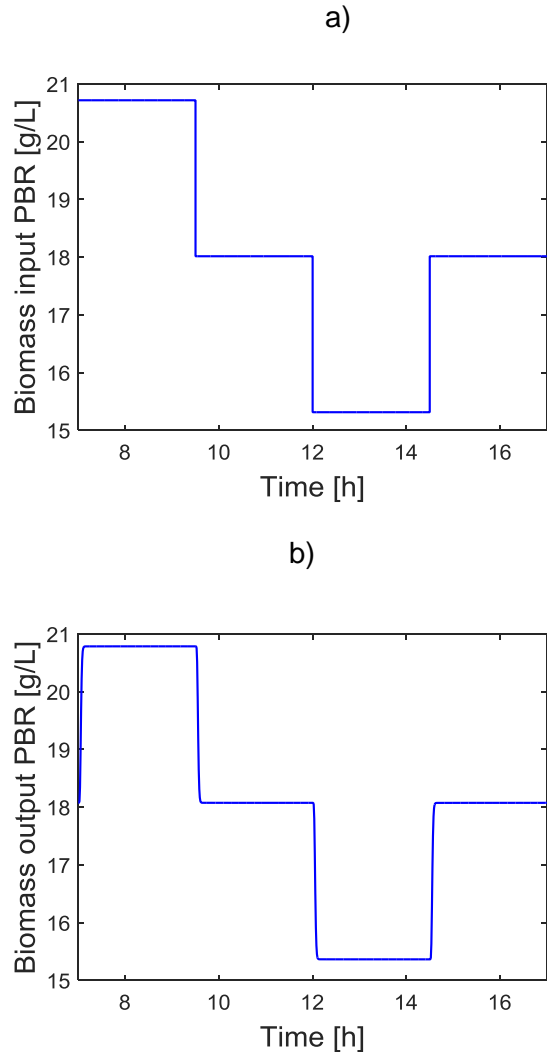


Figure 4-9: Scenario 2, variation of initial biomass a) disturbance b) biomass concentration

Figure 4-10 shows the results of MPC controller. In those is evident that MPC can reach the values of reference, in some intervals of time, in other process values get close to the reference. Those results show the example that in some cases, to have a fixed reference under conditions different of the static optimization can be difficult for the control system, besides of that in some cases this strategy could be incorrect in order to have an optimal performance of the system.

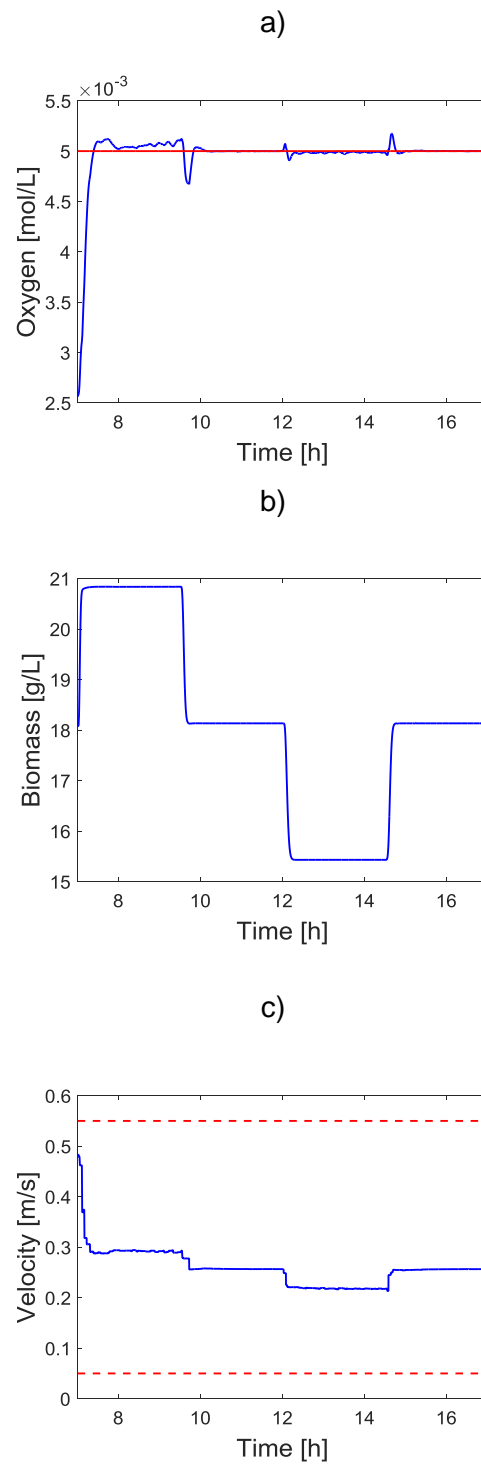


Figure 4-10: MPC results for scenario 2 a) Oxygen concentration b) Biomass concentration c) Velocity

In Figure 4-11 is shown the results of the EMPC for scenario 2 and Figure 4-12 is presented the comparison of MPC controller, EMPC controller and the system in open loop. The biomass concentration reaches higher values than those achieved in open loop, or in the MPC scenario, in some intervals of time. Showing good results for the productivity of the system. Nevertheless, the EMPC controller uses as objective function the energetic function presented previously, which is a non-convex function. Due to it, the EMPC optimization problem can present problems of be unstable or reach local minima.

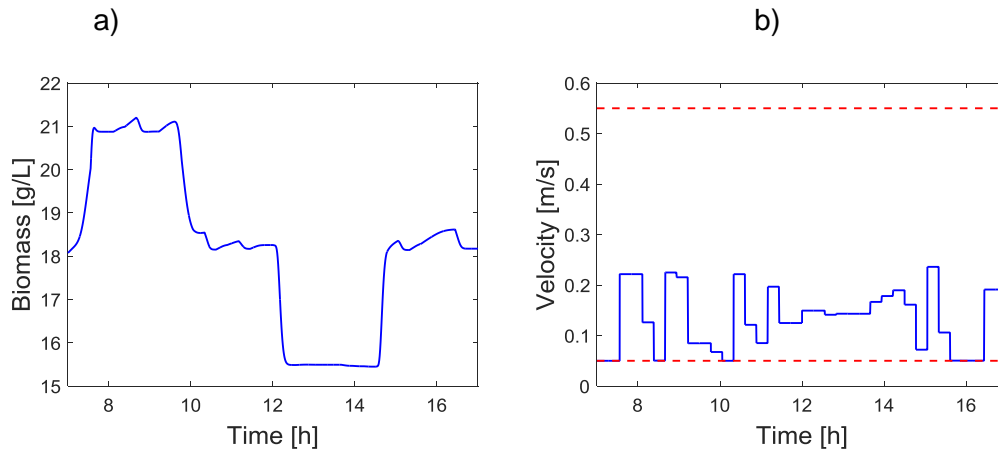


Figure 4-11: EMPC results for scenario 2 a) biomass concentration b) velocity

It is important to highlight that in some intervals, EMPC controller is able to reach higher values for biomass concentration than the reference value of the MPC, which was obtained from a static optimization layer. It means, that for this system under some disturbances a fixed value of the reference calculated with a static optimization may not be adequate in all the conditions.

Besides of that, it is noticeable that EMPC controller shows an important reduction of the flow velocity of the reactor, in comparison to open loop and it showed similar values to MPC controller. It means that the EMPC controller is able to produce similar quantities of biomass that the others, but their control actions lets save a high amount of energy for the operation of PBR. In that way, the EMPC controller is able to manage the system in order to produce a good amount of biomass, and at the same time saving energy as much as possible.

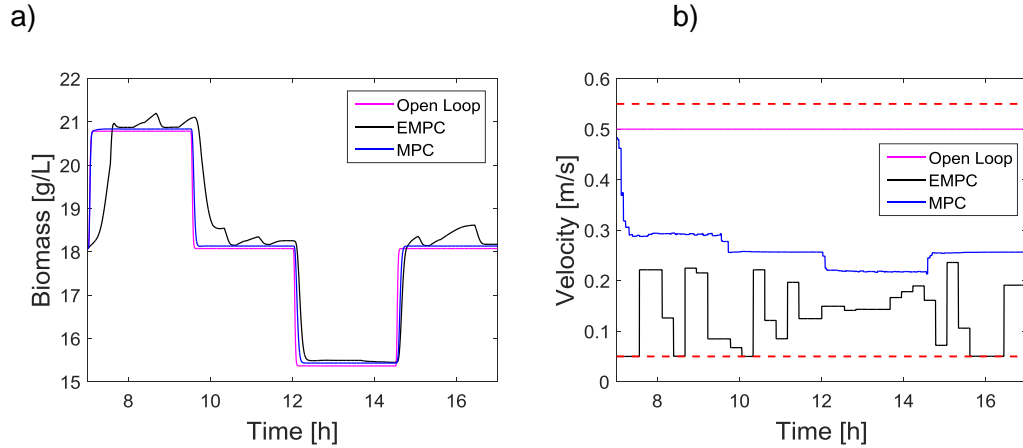


Figure 4-12: Comparison of results for scenario 1 a) biomass concentration b) velocity

4.2.4 Comparison of MPC and EMPC performance.

In order to compare the performance of both control strategies it was necessary to establish some metrics. Energy produced by the system was calculated during the day operation using (4-24). Energy consumed by the system through the pumping system was estimated using (4-25). Finally the difference between both variables was proposed as net energy (4-26), it is important to highlight that the last metric could be the least important, mainly because it is assumed that production and consumption of the system have the same value, and previously it was shown that biomass can have high value applications in different fields. In that sense, a net metric should take into account a specific final application of biomass, and establish adequate weights for biomass and pumping.

$$E_p = \int_{t_0}^{t_f} u_i A (C_{bf} - C_{bi}) \Delta H_b dt \quad (4-24)$$

$$E_c = \int_{t_0}^{t_f} u_i A \Delta P_b dt \quad (4-25)$$

$$E_n = E_p - E_c \quad (4-26)$$

Table 4-1 shows the summary of comparison of scenario 1. In this table it is possible to note that MPC and EMPC strategies can reduce pumping energy, in comparison with the open loop using the optimum velocity suggested in the literature for achieving a good performance in tubular PBR.

Using the equation (4-24) it is possible to calculate an equivalent of energy produced through the biomass in the system. The EMPC controller lets produce 0.27% more energy

in terms of biomass meanwhile MPC controller achieves a reduction of 0.67% in comparison with the optimum operation of the system using a velocity of 0.5 m/s.

Evaluating the equation (4-25) it is possible to estimate the pumping energy required in the system through the flow velocity. The EMPC controller lets to save approximately 95% of pumping energy, meanwhile the MPC controller saves 91%. It is important to note that energy consumption in the system is related to the square of the velocity through the pressure drop, in that sense reductions in velocity produce high reductions in pumping energy.

Table 4-1: Summary first scenario control strategies applied to PBR

Variable	Literature Optimum ($v = 0.5$ m/s)	MPC Control Strategy	Variation (%)	EMPC Control Strategy	Variation (%)
Biomass Energy (BE -Joules)	3.83×10^7	3.81×10^7	-0.67	3.85×10^7	0.27
Biomass Energy (BE -Joules)	2.63×10^6	2.31×10^5	-91.22	1.38×10^5	-94.74
Net Energy (NE -Joules)	3.57×10^7	3.79×10^7	6.0	3.83×10^7	7.28

Finally, the expression (4-26) presents a summary metric between produced energy and required energy in the system, it is the net energy. In terms of net energy, the EMPC improves the economy of the system in 7.28% and MPC improves with 6.0 %. For the first scenario, both control strategies help to improve the economic aspects of the process, in comparison to the optimal value reported for tubular PBR operation and biomass production presented when the velocity is 0.5 m/s.

For the first scenario EMPC controller then is able to produce the best quantities of biomass, expressed as produced energy and the highest value for net energy in the PBR system. Nevertheless, it is important to note that EMPC controller lets save 1.28% more energy of the system in comparison to MPC. It can be interpreted as follows: EMPC controller can produce similar quantities of biomass than MPC controller, but using an amount of energy lower for the pumping system.

Table 4-2 shows the summary of comparison of scenario 2. In this table it is possible to note that MPC and EMPC strategies can reduce pumping energy in comparison with the open loop using a velocity of 0.5 m/s, which is shown in some reports as the optimum velocity for the biomass and operation of tubular PBR.

The EMPC controller reduces in 0.71% the energy produced related to biomass, meanwhile the MPC controller reduces this variable in 0.08% when those are compared with the open loop. The EMPC controller let saves approximately 97% of pumping energy cost, meanwhile the MPC controller saves 88% in comparison with open loop. In terms of net energy, the EMPC improves the economy of the system in 4.8% and MPC increase this variable in 4.7%. For the second scenario, both control strategies help to improve the economic aspects of the process, regarding to the optimal value reported for PBR operation and biomass which is presented using velocities of 0.5 m/s.

For the second scenario EMPC controller then is able to produce almost the same quantities of biomass, and net energy than the MPC controller. According to the results, they produce a little bit less biomass than the optimal value of biomass for the operation of PBR, for open loop ($v = 0.5$ m/s). At the same time, both controllers reduce the pumping energy in a huge amount. Besides of that, it is important to highlight that EMPC controller lets to save 9% more energy in the system when it is compared with the MPC controller. It can be interpreted as follows: EMPC controller can produce the same quantities of MPC controller, but using an amount of energy lower for the pumping system.

Table 4-2: Summary second scenario control strategies applied to PBR

Variable	Literature Optimum ($v = 0.5$ m/s)	MPC Control Strategy	Variation (%)	EMPC Control Strategy	Variation (%)
Biomass Energy (BE -Joules)	4.27×10^7	4.26×10^7	-0.08	4.24×10^7	-0.71
Biomass Energy (BE -Joules)	2.23×10^6	2.77×10^5	-87.55	7.6×10^4	-96.58
Net Energy (NE -Joules)	4.04×10^7	4.23×10^7	4.7	4.23×10^7	4.8

For both scenarios, MPC and EMPC control strategies improve the net energy produced in the system in comparison to an optimal operation of the system proposed in the literature under constant velocity. Both controllers let save a huge amount of energy in the system,

in comparison to open loop; it means: MPC and EMPC improve the overall performance of the PBR under different disturbance conditions, and they produce a good quantity of biomass meanwhile they reduce the pumping energy for the system. EMPC in both scenarios saves 7% more energy than the MPC controller, which could become really important for industrial levels.

Net energy for both scenarios is low, but it is important to highlight that using different cost for microalgae and pumping energy this metric could have very different values. As it was shown previously, once it is established a final application for microalgae, it is possible to fix an economic weight for microalgae from the wide range from 50 €/kg to 150 €/kg, (Fernández et al., 2016).

Results for both controllers are good. Nevertheless, they could be better by means of performing and optimization of tuning parameters. Previously it was mentioned that especially EMPC showed strong dependency with the tuning parameters.

Besides of that, the control strategy and model proposed in this thesis could be improved taking into account more variables (For example: Temperature, oxygen in both phases, dilution rate among many others). Those improvements could let an optimal control of the whole PBR system and increasing the profitability of the system. Also, it could be studied the stability of the EMPC controller, due to the fact that it presents a non-convex objective function. Some of the most important numerical details and comparison are presented in the Annex B as well as some details regarding to the stability of EMPC formulation.

4.2.5 EMPC with Colombian currency in first scenario

In this subsection it is presented a final application of EMPC controller in PBR for the first scenario. The EMPC control strategy presented previously use as variables and objective function some energetic variables. In order to evaluate the controller with Colombian currency Colombian Pesos – COP, it is necessary to modify the optimization problem through the weights in the objective function.

Besides of the variables and expressions presented previously in section 4.1.2 related to the energetic function, it is important to take into account the prices of biomass and energy consumption:

- Biomass selling prices: this variable has a huge range depending of the final application such as: Biofuels, food, secondary metabolites among others (Barsanti & Gualtieri, 2018). That is the reason, it was selected a mid-value for Biomass Price (P_{bi}), it is shown in (4-27).

$$P_{bi} = 1582155.8 \frac{COP}{Kg} \quad (4-27)$$

- Energy consumption price: in the context of Colombia. The price for energy can be obtained from the energetic groups working in this country, for example Codensa (Codensa, 2017) shows in some reports the price. The approximated price of energy (P_e) is shown in (4-28). In the reports there are several values depending of the final application and the type of zone where it is used the energy, it was chosen a value approximately of 224.2 COP/kWh.

$$P_e = 62.27 \times 10^{-5} \frac{COP}{J} \quad (4-28)$$

The EMPC control strategy maintain the same formulation presented previously. Nevertheless, for the biomass term the combustion heat of the microalgae (ΔH_b) must be replaced by Biomass Price (P_{bi}). For the pumping energy, the term has to be multiplied for the value price of energy (P_e). It means, the EMPC has the same structure presented previously, with some variations of constant parameters; it means the weights of terms.

Figure 4-13 shows the results of the EMPC controller using COP weights. In some regions biomass reach values of 18.4 g/l. Velocity profile shows in the majority of operation values lower than 0.1 m/s. The next step is to compare the performance of the MPC and the energetic EMPC formulation with the EMPC in COP.

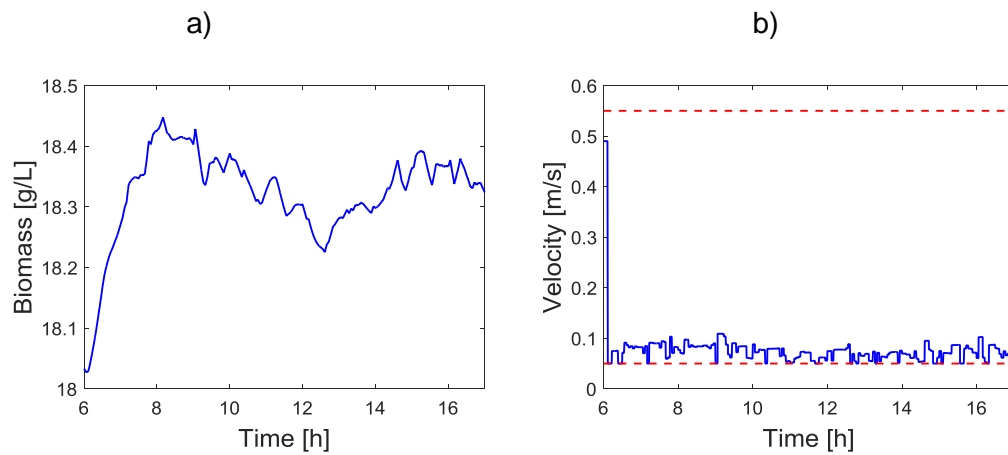


Figure 4-13: Results for first scenario EMPC with COP a) biomass concentration b) velocity

In Figure 4-14 is shown the comparison of all the controllers and the open loop analyzed for first scenario. It is noticeable that biomass for EMPC evaluated with COP present the highest values. At the same time, velocity profile presented for EMPC – COP presents the least values in comparison with the other, it contributes in a huge amount to the economic energetic savings and so on in the economy of the PBR system.

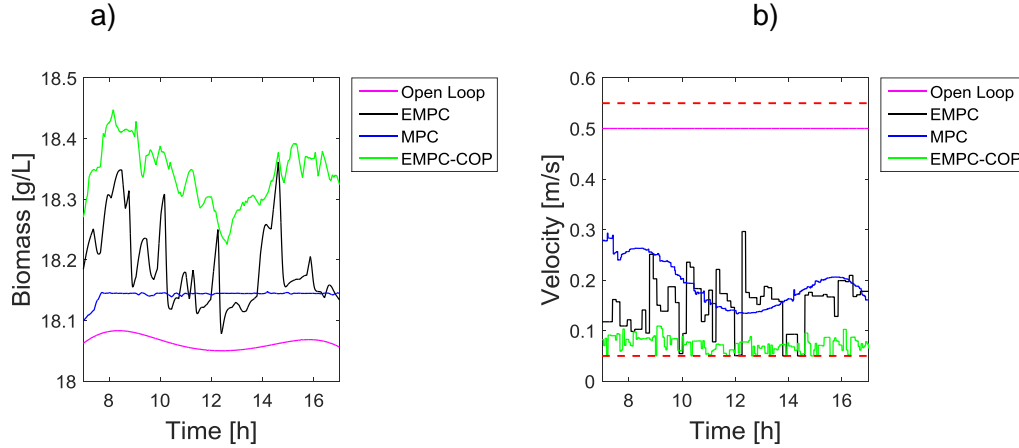


Figure 4-14: Comparison of results for first scenario: Open loop, EMPC, MPC and EMPC - COP a) biomass concentration b) velocity

Finally, it is presented the comparison of results for first scenario through economic metrics. Expressions presented in the section 4.2.4 were modified to include the prices of biomass and pumping energy presented in this section. Those expressions are shown in equations (4-29), (4-30) and (4-31).

$$BP = \int_{t_0}^{t_f} u_i A (C_{bf} - C_{bi}) P_{bi} dt \quad (4-29)$$

$$PC = \int_{t_0}^{t_f} u_i A \Delta P_b P_e dt \quad (4-30)$$

$$NP = BP - PC \quad (4-31)$$

Where Biomass produced is represented by BP , Pumping costs are represent by PC and finally the Net profit in the PBR was calculated as NP shown in (4-31).

Table 4-3 presents the summary for first scenario in COP. In this table it is possible to note that MPC and energetic EMPC and EMPC using COP strategies can reduce pumping energy costs, in comparison with the open loop using the optimum velocity suggested in the literature for achieving a good performance in tubular PBR.

Table 4-3: Summary first scenario in COP: Open loop, EMPC, MPC and EMPC – COP.

Variable	Literature Optimum (v = 0.5 m/s)	MPC Control Strategy	EMPC strategy Energy	EMPC strategy Net profit
Biomass (COP)	3.03×10^6	3.01×10^6	3.02×10^6	2.96×10^6
Pumping Energy (COP)	1.64×10^8	1.44×10^7	6.63×10^6	2.28×10^6
Net profit (COP)	-1.61×10^8	-1.14×10^7	-3.36×10^6	6.78×10^5

Table 4-4 shows the summary of variations for all the controllers compared with the open loop performance. When it is compared the Biomass in the system in COP, all the controllers reduce this value in comparison with the optimum operation of the system using a velocity of 0.5 m/s. MPC reduces biomass in 0.7 %, EMPC energetic strategy reduces in 0.4 % and the EMPC with net profit reduces in 2.6%. Regarding to the pumping energy costs all controllers reduces this requirement; MPC reduces in 91.2%, EMPC with energy reduces 95.9% and EMPC with net profit reduces in 98.61%.

In terms of net profit, all the control strategies improve the net profit for the PBR operation. MPC improves in 92.93%, EMPC with energy in 97.9 and finally the EMPC with net profit presents an improvement more than 100%. It is important to highlight that as it was shown in Table 4-3 and Table 4.4 EMPC with Net profit is the only strategy able to present positive values for net profit variable in COP.

Table 4-4: Variations first scenario: EMPC, MPC and EMPC – COP.

Variable	Literature Optimum (v = 0.5 m/s)	MPC Control Strategy (%)	EMPC strategy Energy (%)	EMPC strategy Net profit (%)
Biomass (COP)	3.03×10^6	-0.67	-0.44	-2.57
Pumping Energy (COP)	1.64×10^8	-91.22	-95.95	-98.61
Net profit (COP)	-1.61×10^8	92.93	97.9	> 100

EMPC net profit strategy produces the least quantities of biomass expressed in COP, at the same time it generates the highest reduction in pumping energy costs, and for net profit this strategy shows a positive value and an improvement higher than 100%. It can be interpreted as follows: EMPC net profit controller can reduce the biomass produced in the system saving a huge amount of energy, in those conditions PBR presents a net profit positive for the system.

Chapter 5: Conclusions and future work

5.1 Conclusions

In this thesis it was proposed and evaluated a new static mixer, whose characteristics let improve agitation and mixing degree, and at the same time reducing energy consumption for pumping of the culture medium. This mixer was used to model the PBR.

The model presented in this thesis combines in simple ways different aspects of the PBR dynamics such as: fluid dynamics, illumination, photosynthesis and mass balances. Besides, it takes into account the LD cycles effect on the behavior of the photosynthesis, and productivity achieved in the PBR. This model can be used in different control strategy, due to its simplicity and that involves the effect of different variables in the productivity of the PBR. This model could be used for optimization purposes.

Here we proposed an objective function which takes into account both aspects for PBR operation: productivity and energy consumption. This function combined with the model can predict in an accurate way optimal region for the PBR.

Both control strategies MPC and EMPC tested in this thesis let reduce in an important amount the pumping energy for the operation of PBR, more than 85% in all cases. Producing almost the same or even better quantities of biomass, with less energy consumption. The proposed EMPC strategy showed a positive economic impact on the PBR operation. EMPC saves 7% more energy than the MPC control strategy.

Evaluating the control strategies in Colombian currency it was found that the EMPC net profit strategy was able to produce positive values for the net profit in PBR operation. It means that an EMPC net profit strategy seems to be a good way to improve the profit in those kinds of systems.

5.2 Products of this thesis

As main products of the thesis, we can list the following items:

- It was developed a research project funded by the government through the Young researchers program: Optimal design strategy of light dark cycles in tubular photobioreactors. In this project it was designed the static mixer used in this model. Also, it was calibrated the main frequencies for the model.
- Conference presentation: in the congressional meeting CCAC 2017 – Cartagena. It was presented an early version of the PBR model in the presentation entitled: Tubular photobioreactor model for light dark cycles control.
- Article 1: Static mixer proposal for tubular photobioreactors to reduce mixing energy consumption and enhance light dark cycles. Status: in preparation. In this document it is presented all the details regarding to the mixer design, and the variables evaluated in order to find the best parameters for the PBR.
- Article 2: Tubular photobioreactor model involving light dark cycles for the microalgae culture control. Status: in preparation. In this document it is presented the whole model used and developed through this research work.

5.3 Future work

In the development of this research work, we found some improvement opportunities regarding to modelling, simulation and control of PBR for this thesis:

- Considering reactants in fluid and gas phase can help to take into account in an accurate way mass transfer inside the reactor.
- Including temperature inside the reactor can provide another control variable for this system, and it would have direct relationship with kinetic growth.
- We focused in agitation and mixing, due to the fact that those take 70% of energy consumption. But taking into account the other 30% energy consumption for the system can lead to improve the performance of the system, such as: aeration, pretreatment of raw materials.
- PBR model and control strategies taking into account other variables can lead to find an optimal operation of the system in a global sense.

References

- Amrit, R. (2011). Optimizing Process Economics in Model Predictive Control.
- Andrade, G. A., Pagano, D. J., Fernández, I., Guzmán, J. L., & Berenguel, M. (2014). Boundary Control of an Industrial Tubular Photobioreactor Using Sliding Mode Control. *IFAC Proceedings Volumes*, 47(3), 4903–4908. <https://doi.org/10.3182/20140824-6-ZA-1003.00900>
- Barsanti, L., & Gualtieri, P. (2018). Is exploitation of microalgae economically and energetically sustainable? *Algal Research*, 31(October 2017), 107–115. <https://doi.org/10.1016/j.algal.2018.02.001>
- Becerra-Celis, G., Hafidi, G., Tebbani, S., Dumur, D., & Isambert, A. (2008). Nonlinear predictive control for continuous microalgae cultivation process in a photobioreactor. *2008 10th International Conference on Control, Automation, Robotics and Vision, ICARCV 2008*, (December), 1373–1378. <https://doi.org/10.1109/ICARCV.2008.4795723>
- Béchet, Q., Shilton, A., & Guieysse, B. (2013). Modeling the effects of light and temperature on algae growth: State of the art and critical assessment for productivity prediction during outdoor cultivation. *Biotechnology Advances*, 31(8), 1648–1663. <https://doi.org/10.1016/j.biotechadv.2013.08.014>
- Benattia, S. E., Tebbani, S., & Dumur, D. (2015). Hierarchical Control Strategy based on Robust MPC and Integral Sliding mode - Application to a Continuous Photobioreactor. *IFAC-PapersOnLine*, 48(23), 212–217. <https://doi.org/10.1016/j.ifacol.2015.11.285>
- Benattia, S. E., Tebbani, S., Dumur, D., & Selis, D. (2014). Robust Nonlinear Model Predictive Controller Based on Sensitivity Analysis - Application to a Continuous Photobioreactor, 1705–1710. <https://doi.org/10.1109/CCA.2014.6981558>
- Bitog, J. P., Lee, I. B., Lee, C. G., Kim, K. S., Hwang, H. S., Hong, S. W., ... Mostafa, E.

- (2011). Application of computational fluid dynamics for modeling and designing photobioreactors for microalgae production: A review. *Computers and Electronics in Agriculture*, 76(2), 131–147. <https://doi.org/10.1016/j.compag.2011.01.015>
- Brennan, L., & Owende, P. (2010). Biofuels from microalgae-A review of technologies for production, processing, and extractions of biofuels and co-products. *Renewable and Sustainable Energy Reviews*, 14(2), 557–577. <https://doi.org/10.1016/j.rser.2009.10.009>
- Cesário, M. T., da Fonseca, M. M. R., Marques, M. M., & de Almeida, M. C. M. D. (2018). Marine algal carbohydrates as carbon sources for the production of biochemicals and biomaterials. *Biotechnology Advances*, 36(3), 798–817. <https://doi.org/10.1016/j.biotechadv.2018.02.006>
- Chen, Y., Xu, C., & Vaidyanathan, S. (2018). Microalgae: a robust “green bio-bridge” between energy and environment. *Critical Reviews in Biotechnology*, 38(3), 351–368. <https://doi.org/10.1080/07388551.2017.1355774>
- Cheng, W., Huang, J., & Chen, J. (2014). Computational fluid dynamics simulation of mixing characteristics and light regime in tubular photobioreactors with novel static mixers. *Journal of Chemical Technology and Biotechnology*, 91(2), 327–335. <https://doi.org/10.1002/jctb.4560>
- COMSOL. (2012). Comsol Multiphysics User’s Guide. *The Heat Transfer Branch*, 709–745, The Heat Transfer Branch.
- COMSOL. (2013). The Particle Tracing Module User’s Guide.
- Eilers, P. H. C., & Peeters, J. C. H. (1988). A model for the relationship between light intensity and the rate of photosynthesis in phytoplankton. *Ecological Modelling*, 42(3–4), 199–215. [https://doi.org/10.1016/0304-3800\(88\)90057-9](https://doi.org/10.1016/0304-3800(88)90057-9)
- Ellis, M., Durand, H., & Christofides, P. D. (2014). A tutorial review of economic model predictive control methods. *Journal of Process Control*, 24(8), 1156–1178. <https://doi.org/10.1016/j.jprocont.2014.03.010>
- Fernández, I., Ación, F. G., Berenguel, M., Guzmán, J. L., Andrade, G. A., & Pagano, D. J. (2014). A lumped parameter chemical-physical model for tubular photobioreactors. *Chemical Engineering Science*, 112, 116–129. <https://doi.org/10.1016/j.ces.2014.03.020>
- Fernández, I., Berenguel, M., Guzmán, J. L., Ación, F. G., Andrade, G. A., & Pagano, D. J. (2015). Hierarchical Non-linear Control of a Tubular Photobioreactor. *IFAC-*

- PapersOnLine*, 48(23), 224–229. <https://doi.org/10.1016/j.ifacol.2015.11.287>
- Fernández, I., Berenguel, M., Guzmán, J. L., Ación, F. G., de Andrade, G. A., & Pagano, D. J. (2016). Hierarchical control for microalgae biomass production in photobioreactors. *Control Engineering Practice*, 54, 246–255. <https://doi.org/10.1016/j.conengprac.2016.06.007>
- Forbes, M. G., Patwardhan, R. S., & Gopaluni, R. B. (2015). Model predictive control in industry challenges and opportunities. *Advanced Control of Chemical Processes*, 532–539.
- Forbes, M. G., Patwardhan, R. S., Hamadah, H., & Gopaluni, R. B. (2015). Model predictive control in industry: Challenges and opportunities. *IFAC-PapersOnLine*, 28(8), 531–538. <https://doi.org/10.1016/j.ifacol.2015.09.022>
- García C., R. (2012). Tesis Doctoral: Producción de biomasa de microalgas rica en carbohidratos acoplada a la eliminación fotosintética de dióxido de carbono. *Universidad de Sevilla*.
- García, J., Fernández-Anaya, G., Vargas-Villamil, F. D., & Orduña, E. (2010). ESTRUCTURA DE CONTROL JERARQUICO APLICADA A UN REACTOR DE AMONIACO, TIPO TUBULAR, CON ENFRIAMIENTO INTERMEDIO. *Revista Mexicana de Ingeniería Química*, 9.
- Gargano, I., Olivieri, G., Spasiano, D., Andreozzi, R., Pollio, A., Marotta, R., ... Marzocchella, A. (2015). Kinetic characterization of the photosynthetic reaction centres in microalgae by means of fluorescence methodology. *Journal of Biotechnology*, 212, 1–10. <https://doi.org/10.1016/j.jbiotec.2015.07.009>
- Giwa, A., Adeyemi, I., Dindi, A., Lopez, C. G. B., Lopresto, C. G., Curcio, S., & Chakraborty, S. (2018). Techno-economic assessment of the sustainability of an integrated biorefinery from microalgae and *Jatropha*: A review and case study. *Renewable and Sustainable Energy Reviews*, 88(February 2017), 239–257. <https://doi.org/10.1016/j.rser.2018.02.032>
- Gómez-pérez, C. A., Espinosa, J., Ruiz, L. C. M., & Boxtel, A. J. B. Van. (2015). CFD simulation for reduced energy costs in tubular photobioreactors using wall turbulence promoters. *ALGAL*, 12, 1–9. <https://doi.org/10.1016/j.algal.2015.07.011>
- Gómez-Pérez, C. A., Espinosa Oviedo, J. J., Montenegro Ruiz, L. C., & van Boxtel, A. J. B. (2017). Twisted tubular photobioreactor fluid dynamics evaluation for energy consumption minimization. *Algal Research*, 27, 65–72. <https://doi.org/10.1016/j.algal.2017.08.019>

-
- González-Delgado, Á.-D., & Kafarov, V. (2011). MICROALGAE BASED BIOREFINERY: ISSUES TO CONSIDER. *CT&F - Ciencia, Tecnología y Futuro*, 4(4), 5–22. Retrieved from http://www.scielo.org.co/scielo.php?script=sci_arttext&pid=S0122-53832011000200001
- Gutierrez-Wing, M. T., Silaban, A., Barnett, J., & Rusch, K. A. (2014). Light irradiance and spectral distribution effects on microalgal bioreactors. *Engineering in Life Sciences*, 14(6), 574–580. <https://doi.org/10.1002/elsc.201300152>
- Han, B. P. (2001). Photosynthesis-irradiance response at physiological level: a mechanistic model. *Journal of Theoretical Biology*, 213(2), 121–127. <https://doi.org/10.1006/jtbi.2001.2413>
- Hartmann, P., Béchet, Q., & Bernard, O. (2014). The effect of photosynthesis time scales on microalgae productivity. *Bioprocess and Biosystems Engineering*, 37(1), 17–25. <https://doi.org/10.1007/s00449-013-1031-2>
- Harun, R., Singh, M., Forde, G. M., & Danquah, M. K. (2010). Bioprocess engineering of microalgae to produce a variety of consumer products. *Renewable and Sustainable Energy Reviews*, 14(3), 1037–1047. <https://doi.org/10.1016/j.rser.2009.11.004>
- Heidarinejad, M., Liu, J., & Christofides, P. D. (2011). Lyapunov-based economic model predictive control of nonlinear systems. *American Control Conference*, 5195–5200. <https://doi.org/10.1109/ACC.2014.6859472>
- Holkar, K. S., & Waghmare, L. M. (2010). An overview of model predictive control. *International Journal of Control and Automation*, 3(4), 7.
- Huang, J., Feng, F., Wan, M., Ying, J., Li, Y., Qu, X., ... Li, W. (2015). Improving performance of flat-plate photobioreactors by installation of novel internal mixers optimized with computational fluid dynamics. *Bioresource Technology*, 182, 151–159. <https://doi.org/10.1016/j.biortech.2015.01.067>
- Huang, J., Kang, S., Wan, M., Li, Y., Qu, X., Feng, F., ... Li, W. (2014). Numerical and experimental study on the performance of flat-plate photobioreactors with different inner structures for microalgae cultivation. *Journal of Applied Phycology*. <https://doi.org/10.1007/s10811-014-0281-y>
- Janssen, M., Tramper, J., Mur, L. R., & Wijffels, R. H. (2003). Enclosed outdoor photobioreactors: light regime, photosynthetic efficiency, scale-up, and future prospects. *Biotechnology and Bioengineering*, 81(2), 193–210. <https://doi.org/10.1002/bit.10468>

- Jaramillo, G. Y., & Bustamante, E. M. (2005). Los balances energéticos en la producción agropecuaria. *Energetica*, 33, 73–90.
- Kimiaghalam, B., Ahmadzadeh, A., Homaifar, A., Sayarrodsari, B., & Technologies, P. (2003). A Purely Model Predictive Control For A Marginally Stable System, 4293–4298.
- Lee, J. (2014). *Linear and Nonlinear Distributed Economic Model Predictive Control*. Imperial College London of Science. <https://doi.org/10.1007/978-1-4471-5102-9>
- Lehr, F., & Posten, C. (2009). Closed photo-bioreactors as tools for biofuel production. *Current Opinion in Biotechnology*, 20(3), 280–285. <https://doi.org/10.1016/j.copbio.2009.04.004>
- Luo, H. P., & Al-Dahhan, M. H. (2004). Analyzing and Modeling of Photobioreactors by Combining First Principles of Physiology and Hydrodynamics. *Biotechnology and Bioengineering*, 85(4), 382–393. <https://doi.org/10.1002/bit.10831>
- Marquez, A., Gomez, C., Deossa, P., & Espinosa, J. (2011). Infinite Horizon MPC and model reduction applied to large scale chemical plant. *2011 IEEE 9th Latin American Robotics Symposium and IEEE Colombian Conference on Automatic Control, LARC 2011 - Conference Proceedings*, (65). <https://doi.org/10.1109/LARC.2011.6086842>
- Marquez, A., Patiño, J., & Espinosa, J. (2014). Min-Max Economic Model Predictive Control. *53rd IEEE Conference on Decision and Control Conference Proceedings*, (1994), 1–9. <https://doi.org/10.1007/978-1-4471-5102-9>
- Marshall, J. S., & Huang, Y. (2010). Simulation of light-limited algae growth in homogeneous turbulence. *Chemical Engineering Science*, 65(12), 3865–3875. <https://doi.org/10.1016/j.ces.2010.03.036>
- Mayne, D. Q. (2014). Model predictive control: Recent developments and future promise. *Automatica*, 50(12), 2967–2986. <https://doi.org/10.1016/j.automatica.2014.10.128>
- Medianu, S., & Popescu, D. (2012). SUPERVISORY CONTROL FOR ETHYLENE PRODUCTION IN PETROCHEMICAL INSTALLATIONS, 230–232.
- Merchuk, J. C., & Wu, X. (2003). Modeling of photobioreactors: Application to bubble column simulation. *Journal of Applied Phycology*, 15, 163–169. <https://doi.org/10.1023/A:1023879619535>
- Minasidis, V., & Johannes, J. (2013). Economic plantwide control : Automated controlled variable selection for a reactor-separator-recycle process.
- Molina, E., Fernández, J., Acien, F. G., & Chisti, Y. (2001). Tubular photobioreactor design for algal cultures. *Journal of Biotechnology*, 92(2), 113–131.

- [https://doi.org/10.1016/S0168-1656\(01\)00353-4](https://doi.org/10.1016/S0168-1656(01)00353-4)
- Molina Grima, E., Acién Fernández, F. G., García Camacho, F., & Chisti, Y. (1999). Photobioreactors: light regime, mass transfer, and scaleup. *Journal of Biotechnology*, 70(1–3), 231–247.
- Molina Grima, E., García Camacho, F., Pérez Sánchez, J. A., Acién Fernández, F. G., & Fernández Sevilla, J. M. (1997). Evaluation of photosynthetic efficiency in microalgal cultures using averaged irradiance. *Enzyme and Microbial Technology*, 21, 375–381.
- Norsker, N.-H., Barbosa, M. J., Vermuë, M. H., & Wijffels, R. H. (2011). Microalgal production--a close look at the economics. *Biotechnology Advances*, 29(1), 24–7. <https://doi.org/10.1016/j.biotechadv.2010.08.005>
- Norsker, N. H., Barbosa, M. J., Vermuë, M. H., & Wijffels, R. H. (2011). Microalgal production - A close look at the economics. *Biotechnology Advances*, 29(1), 24–27. <https://doi.org/10.1016/j.biotechadv.2010.08.005>
- Park, K., & Lee, C. (2000). Optimization of algal photobioreactors using flashing lights. *Biotechnology and Bioprocess Engineering*, 5(3), 186–190.
- Pawłowski, A., Guzmán, J. L., Berenguel, M., Acién, F. G., & Dormido, S. (2018). Application of predictive feedforward compensator to microalgae production in a raceway reactor: A simulation study. *Energies*, 11(1). <https://doi.org/10.3390/en11010123>
- Perner-Nochta, I., & Posten, C. (2007). Simulations of light intensity variation in photobioreactors. *Journal of Biotechnology*, 131(3), 276–285. <https://doi.org/10.1016/j.jbiotec.2007.05.024>
- Posten, C. (2009). Design principles of photo-bioreactors for cultivation of microalgae. *Engineering in Life Sciences*, 9(3), 165–177. <https://doi.org/10.1002/elsc.200900003>
- Posten, C., & Schaub, G. (2009). Microalgae and terrestrial biomass as source for fuels-A process view. *Journal of Biotechnology*, 142(1), 64–69. <https://doi.org/10.1016/j.jbiotec.2009.03.015>
- Richalet, J., Rault, A., Testud, J. L., & Papon, J. (1978). Model predictive heuristic control. Applications to industrial processes. *Automatica*, 14(5), 413–428. [https://doi.org/10.1016/0005-1098\(78\)90001-8](https://doi.org/10.1016/0005-1098(78)90001-8)
- Salguero-rodíguez, Y., Gómez-perez, C. A., José, J., & Oviedo, E. (2017). Tubular photobioreactor model for light – dark cycles control. *2017 IEEE 3rd Colombian Conference on Automatic Control, CCAC 2017 - Conference Proceedings*, 1–6.

- Sandoz, D. J., Desforges, M. J., Lennox, B., & Goulding, P. R. (2000). Algorithms for industrial model predictive control. *Computing & Control Engineering Journal*, 11(3), 125–134. <https://doi.org/10.1049/cce:20000306>
- Santander, O., Elkamel, A., & Budman, H. (2016). Economic model predictive control of chemical processes with parameter uncertainty. *Computers and Chemical Engineering*, 95, 10–20. <https://doi.org/10.1016/j.compchemeng.2016.08.010>
- Singh, R. N., & Sharma, S. (2012). Development of suitable photobioreactor for algae production - A review. *Renewable and Sustainable Energy Reviews*, 16(4), 2347–2353. <https://doi.org/10.1016/j.rser.2012.01.026>
- Soman, A., & Shastri, Y. (2015). Optimization of novel photobioreactor design using computational fluid dynamics. *Applied Energy*, 140, 246–255. <https://doi.org/10.1016/j.apenergy.2014.11.072>
- Su, Z., Kang, R., Shi, S., Cong, W., & Cai, Z. (2010). Study on the destabilization mixing in the flat plate photobioreactor by means of CFD. *Biomass and Bioenergy*, 34(12), 1879–1884. <https://doi.org/10.1016/j.biombioe.2010.07.025>
- Suh, I. S., & Lee, C.-G. (2003). Photobioreactor engineering: Design and performance. *Biotechnology and Bioprocess Engineering*, 8(6), 313–321. <https://doi.org/10.1007/BF02949274>
- Takache, H., Pruvost, J., & Marec, H. (2015). Investigation of light/dark cycles effects on the photosynthetic growth of *chlamydomonas reinhardtii* in conditions representative of photobioreactor cultivation. *Algal Research*, 8, 192–204. <https://doi.org/10.1016/j.algal.2015.02.009>
- Tran, T., Ling, K.-V., & Maciejowski, J. M. (2014). Economic Model Predictive Control - A Review. *The 31st International Symposium on Automation and Robotics in Construction and Mining (ISARC 2014)*, (Isarc).
- Uyar, B., & Kapucu, N. (2015). Passive temperature control of an outdoor photobioreactor by phase change materials. *Journal of Chemical Technology and Biotechnology*, 90(5), 915–920. <https://doi.org/10.1002/jctb.4398>
- Wu, L. B., Li, Z., & Song, Y. Z. (2010). Hydrodynamic conditions in designed spiral photobioreactors. *Bioresource Technology*, 101(1), 298–303. <https://doi.org/10.1016/j.biortech.2009.08.005>
- Wu, X., & Merchuk, J. C. (2001). A model integrating fluid dynamics in photosynthesis and photoinhibition processes. *Chemical Engineering Science*, 56(11), 3527–3538. [https://doi.org/10.1016/S0009-2509\(01\)00048-3](https://doi.org/10.1016/S0009-2509(01)00048-3)

-
- Wu, X., & Merchuk, J. C. (2002). Simulation of algae growth in a bench-scale bubble column reactor. *Biotechnology and Bioengineering*, *80*(2), 156–168. <https://doi.org/10.1002/bit.10350>
- Yan, H., Guan, C., Jia, Y., Huang, X., & Yang, W. (2018). Mixing characteristics, cell trajectories, pressure loss and shear stress of tubular photobioreactor with inserted self-rotating helical rotors. *Journal of Chemical Technology and Biotechnology*, *93*(5), 1261–1269. <https://doi.org/10.1002/jctb.5484>
- Zhang, Q., Wu, X., Xue, S., Liang, K., & Cong, W. (2013). Study of hydrodynamic characteristics in tubular photobioreactors. *Bioprocess and Biosystems Engineering*, *36*(2), 143–150. <https://doi.org/10.1007/s00449-012-0769-2>
- Zhang, T. (2013). Dynamics of fluid and light intensity in mechanically stirred photobioreactor. *Journal of Biotechnology*, *168*(1), 107–116. <https://doi.org/10.1016/j.jbiotec.2013.07.007>
- Zijffers, J. F., Schippers, K. J., Zheng, K., Janssen, M., & Tramper, J. (2010). Maximum Photosynthetic Yield of Green Microalgae in Photobioreactors, 708–718. <https://doi.org/10.1007/s10126-010-9258-2>

A. Annex A: Pressure drop

In this thesis it was proposed a new energetic function, in chapter 4, which takes into account the pressure drop in order to calculate the economic benefit of the photobioreactor. It is required an expression for the pressure drop (ΔP_b) as function of velocity (v_b) in order to calculate the pumping energy. Pressure drop for different velocities was taken from CFD calculations showed previously and it is presented in the figure 6-1.

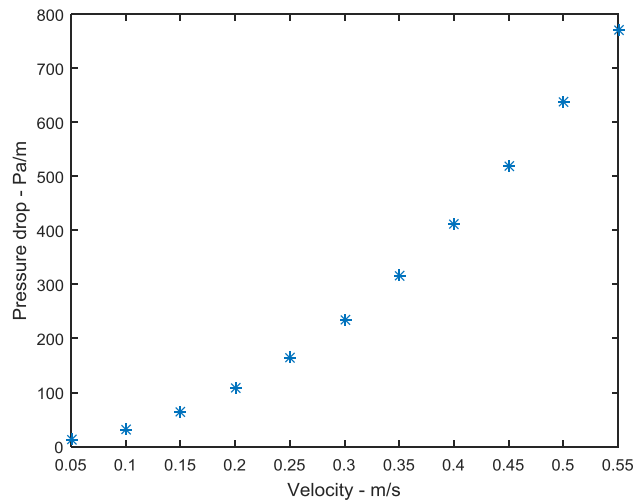


Figure 6-1: Pressure drop as function of velocity

It is well known that pressure drop is directly proportional to the square of velocity head, due to it, we plotted pressure drop versus the square of the velocity, and it is shown in figure 6-2. In that figure, it is evident a linear relationship between pressure drop per length and the square of the velocity, expression (6-1) can be used for further calculations related to the economic benefit of the photobioreactor.

$$\Delta P_b = 2525.7 \times v_b^2 + 6.7065 \quad (6-1)$$

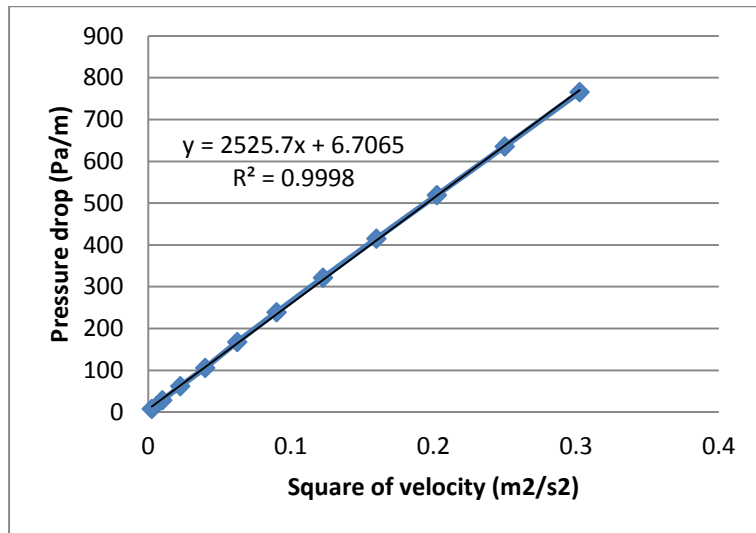


Figure 6-2: Pressure drop as function of square of velocity

B. Annex B: Numerical details and comparison of control strategies

In this thesis it was presented the application of some control strategies in PBR. In this annex it is explained more about the numerical details and solution algorithm as well as some comparison and discussion about controllers.

Controllers start their work after the system reaches the steady state under certain conditions. Due to it, the first step is to simulate the dynamic of the system until it reaches the equilibrium. It was simulated coupling in a system of ordinal differential equations – ODE all the equations presented for the model of PBR and the kinetic model in section 3.1. Light dark cycles model presented in 3.1.4 was coupled inside the kinetic model equations in order to obtain the effect over the specific growth rate. ODE system was solved through the Matlab function “ode45”, which works using a Runge-Kutta method of solution. It was activated the setting to non-negative solutions for “ode45” mainly due to the fact that some variables could be close zero values and some numerical errors and approximation can lead to negative values. Negative values should be avoided in this simulation because physically it is not possible to achieve negative values for concentrations. After that, it was saved the final conditions for the states of the system, they are used in further steps due to the fact that all controllers will start to work from the steady state.

For the MPC controller it was created a Matlab function, which evaluates the expressions for the MPC controller presented in 4.1.1. The optimization problem was solved through the Matlab function “fmincon” which is useful to find the minimum of constrained nonlinear multivariable problems. Algorithm sequential quadratic programming – SQP was selected as algorithm method in the “fmincon”, due to the fact that MPC optimization problem present constrains and a quadratic function. Then the optimization algorithm finds the best control action for the system the model is simulated as showed previously with that control action. This process is repeated as many times as it is needed to simulate all the scenarios.

In the EMPC controller it was built a Matlab function, which evaluates the expressions for the EMPC controller presented in 4.1.3. The optimization problem was solved in a similar

way to the MPC problem with the Matlab function “fmincon”. Algorithm sequential quadratic programming – SQP was selected as algorithm method in the “fmincon”, due to the fact that EMPC optimization problem present constrains and a nonlinear objective function, for those cases SQP algorithm has shown good results. After the optimization process finds the best control action for the system the model is simulated as showed previously with the control action. This process is repeated as many times as it is needed to simulate all the scenarios.

For EMPC expressed in COP it was built a Matlab function, which evaluates the expressions for EMPC in COP presented in 4.2.5. The formulation of EMPC in COP is similar to the EMPC presented in section 4.1.3, the only difference is that the weights of the multiobjective optimization problem were changed. The optimization problem was solved in a similar way to the EMPC problem with the Matlab function “fmincon”. After the optimization process finds the best control action for the system the model is simulated as showed previously with the control action. This process is repeated as many times as it is needed to simulate all the scenarios.

Table 6-1 summarizes the simulation time during 12 h of simulation of scenarios, from 6 am to 6 pm. MPC is the fastest with 800 s. EMPC presents a time approximately 30% higher than MPC simulation. EMPC in COP showed a simulation time of 1050 s, this value is similar to the EMPC Energy simulation, and it is approximately 25% higher than MPC simulation. This is a metric about the numerical complexity of the problem, in which it is possible to appreciate that the MPC is the easiest and fastest to solve.

Table 6-1: Summary first scenario in COP: Open loop, EMPC, MPC and EMPC – COP.

MPC	EMPC Energy	EMPC in COP
800 s	1092 s	1050 s

Finally, in this section, it is presented the discussion related to the stability of the EMPC controllers presented here. For both EMPC controllers the objective function is non-convex function because of that the EMPC optimization problem can present difficult of unstable or reach local minima. In that sense there are two ways to try to solve the problem of non-convexity of objective function. Those are:

- As it is possible to see, the term T1 presented in 4.1.3 is with a negative sign which affects the convexity. An alternative is to replace the T1 using a new term in which the EMPC optimization tracks a reference, avoiding the minus sign. The reference should be calculated or fixed as an ideal reference in which the PBR system should have a good performance. So, the objective function could be described as a convex problem.
- Another way to help the optimization problem is to replace the non-convex objective function with a linearized approximation of the objective function using the gradient of the non-convex function. It means, describe the non-convex objective function as a linear convex function.

Those are some ways to help the optimization problem and so, improve the stability and performance of the controllers EMPC.