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SIMULATION OF THE BIOMASS AND LIPID PRODUCTION PROCESS FROM *PARACHLORELLA SP*.

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Microalgae are a renewable source of biomass for the production of third-generation biofuels that have aroused great interest worldwide because of their rapid growth and ability to fix atmospheric CO2. Additionally, they are capable of accumulating oil in proportions that can exceed 60% of the dry weight, which makes them attractive for biodiesel production. This project aims to evaluate the simulation of the biomass and oil production process using the alga *Parachlorella sp*. via ASPEN software. The simulation is based on the fixation of CO2 by algae, which, via their cellular metabolism, transforms it into oil, which is then extracted and transesterified into biodiesel. The simulation demonstrated significant biomass growth, since a mass flow of 1000 kg/h of *Parachlorella sp*. was entered and 336.435 kg/h of biomass was produced, taking into account the necessary nutrients such as water, CO2, oxygen, hydrogen, and carbon sources and a nitrogen source. In addition, a stoichiometric reaction for the conversion of CO2 into tripalmitic oil was generated, resulting in 224.809 kg/h CO2. Through this simulation, a new perspective of decarbonization, biomass generation and, in some cases, biofuels can be developed.

1. Introduction

Human actions, primarily the burning of fossil fuels such as coal, oil and gas, have driven climate change since the 19th century, generating 75% of greenhouse gas (GHG) emissions and approximately 90% of carbon dioxide (CO2) emissions (Huang et al., 2012). This has raised the average global temperature by 1.1°C compared with the 1850–1900 period (IPCC, 2023), releasing large amounts of CO2 into the atmosphere. In 2019, atmospheric concentrations of CO2 reached 410 parts per billion, an increase of 47% since 1750 (IPCC,2023). Thus, to avoid the negative impacts of climate change, emissions must be reduced by approximately 50% by 2030, and net zero must be achieved by 2050.

For this reason, renewable energy applications have generated interest in sustainable development, energy security, depletion of fossil fuels and nonrenewable resources (Amjith & Bavanish, 2022), with biofuels and biomass being the only renewable energy sources capable of directly replacing them (Mahmood et al., 2022). For some years, biofuels whose raw material is of biological origin have been produced, and the first generation of biofuels is the most common form of production, which uses vegetable oils derived from edible biomass as raw material. The second generation of biofuels is obtained from nonedible oils, industrial waste, and agricultural and forestry waste (Escobedo & Calderón, 2021). Finally, third-generation biofuels from microalgae are considered a technically viable alternative energy resource (Abdelsalam et al., 2019).

The third generation of biofuels from microalgae has emerged as a sustainable alternative to traditional biodiesel feedstocks (Abdelsalam et al., 2019; Escobedo & Calderón, 2021). Microalgae are unicellular microorganisms that are easy to cultivate and have the ability to fix atmospheric CO2 while reproducing rapidly, so they are promising prospects for effectively sequestering carbon and mitigating GHG emissions (Pekkoh et al., 2024). In addition, they contain more than 80% organic matter, allowing carbon to be stored in the form of lipids, carbohydrates, proteins, vitamins and fatty acids to produce biodiesel and bioethanol (Escobedo & Calderón, 2021; Mousavi et al., 2022; Wang et al., 2020; Zebian et al., 2024). Because they are in aqueous media, they can absorb large amounts of CO2 and nutrients, and through photosynthesis, they convert solar energy into microalgal biomass (Escobedo & Calderón, 2021).

For their growth, they need three main components, which are sources of light, water and carbon (Rizwan et al., 2018); however, factors such as temperature, nutrients (mainly nitrogen and phosphorus), pH and salinity must also be considered (Debnath et al., 2021; Escobedo & Calderón, 2021; Johnson, 2012; Mahmood et al., 2022). Owing to their remarkable adaptability in their habitat, they can grow in wastewater, including sanitary, industrial and agro-industrial wastewater (Debnath et al., 2021; Wu et al., 2014). The oil content of microalgae (20% - 50%) (Escobedo & Calderón, 2021; Johnson, 2012) is higher than that of other oil sources, producing between 15 and 300 times more oil for biodiesel production than traditional crops per surface area (Saifullah et al., 2014; Johnson, 2012).

The simulation of the production process is highly complex due to the various reactions occurring within the cells, and since ASPEN was developed for chemical reactions, simulating biochemical reactions is particularly challenging. In this work, the simulation of the biomass and lipid production process from *Parachlorella sp*. will be carried out, thus establishing the stages required for the process, the operating conditions of each of these stages and, finally, determining the material and energy balances.

1. Materials and methods

2.1. Biomass characteristics

To simulate the behavior of *Parachorella* sp. in the ASPEN simulator, it was necessary to model the biomass as a nonconventional component. For this purpose, proximate and ultimate analyses of *C. vulgaris* were used, as shown in Table 1, including its percentages of ash, volatile matter (VM), fixed carbon (FC), and moisture (M):

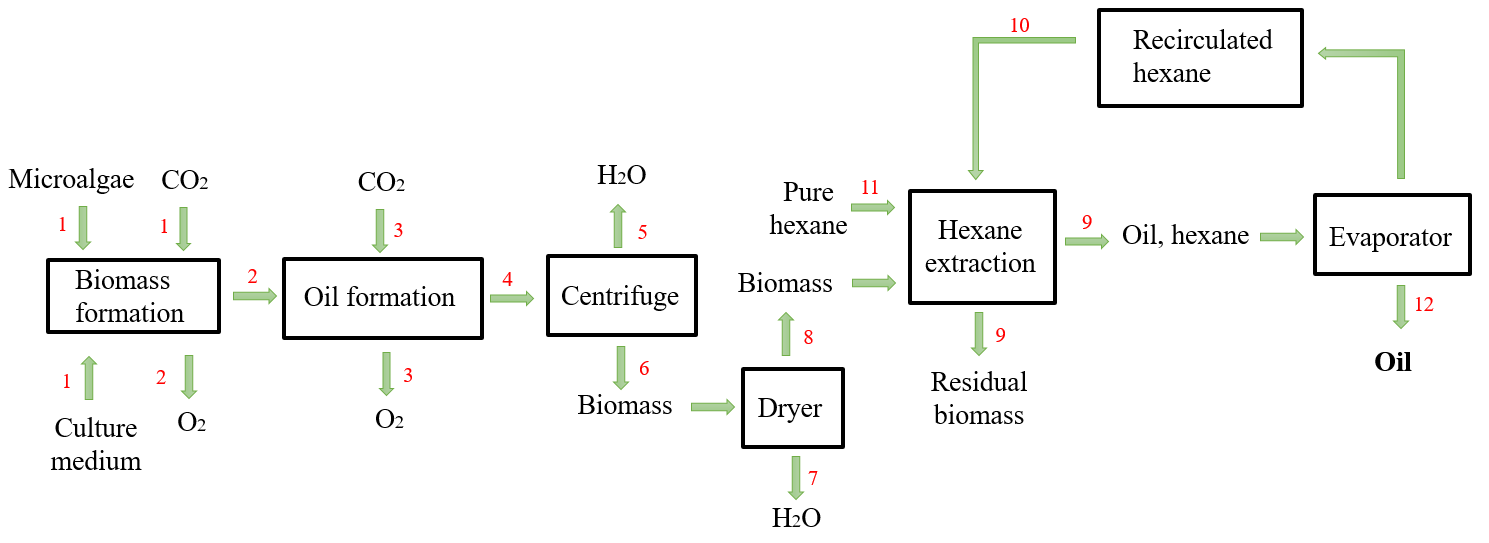
*Table 1. Proxanal and ultimate (C, H, O, N, S) analysis of Chlorella vulgaris*

|  |  |
| --- | --- |
| Characteristic | (Magalhães et al., 2022) |
| Moisture | 6.18 |
| Volatile matter | 66.56 |
| Ash | 15.64 |
| Fixed carbon | 11.62 |
| C | 43 |
| H | 6.77 |
| O | 27.95 |
| N | 6.64 |
| S | 0 |

**2.2. Aspen Plus Modeling**

The biomass production process from *Parachlorella sp*. consists of 5 main stages: 1) cultivation, 2) harvesting, 3) drying, 4) oil extraction and 5) obtaining residual biomass (Escobedo & Calderón, 2021; Maldonado Barraza, 2011). Figure 1 shows a diagram of the process with 5 stages. This process shows that the production of oil by *Parachlorella* sp. is complex because it includes different biochemical reactions (Table 3). CO2 must be dissolved in water for incorporation into the cell, and the solubility of CO2 is approximately 1.45 g CO2/L at 30°C (temperature of the culture). Once the CO2 is dissolved in the water, an equilibrium is reached such that the CO2 is transformed into carbonic acid (H2CO3), carbonate (CO3 2-) or bicarbonate (HCO3 1-), depending on the pH of the solution. At a pH of 7.0, most carbonic acid is converted into bicarbonate and CO2, and as shown in Table 3, the presence of both substances was considered. CO2 is transformed into biomass and oil following the Calvin cycle, the glycolysis pathway, the Krebs cycle, the tricarboxylic acid pathway, the acetyl-CoA carboxylase and fatty acid synthase pathway and triglyceride synthase (Table 2). The global reaction was considered for the simulation in the reactor in two stages: biomass and oil formation using a stoichiometric reactor.

The simulation was developed for a flow of 1000 kg/h of CO2 entering the biomass reactor and for 625 kg/h of CO2 entering the oil reactor (Figure 1). From this quantity of CO2, the other substances involved in the reactions were calculated according to the reactions (Table 2). The stoichiometric reaction given by (Yu & Lu, 2019)​ was used, where an autotrophic microalga is used in a steady state, and this was adjusted for the generation of biomass on a large scale, thus obtaining Eq (1). The thermodynamic model used in Aspen Plus was a Peng-Robinson model. A centrifuge was used to separate the liquids from the solids. At the end of the process, an extraction column with hexane was used to extract the oil from the biomass. Finally, the evaporated hexane is recovered and recirculated so that it enters the extraction column again (Gurreri et al., 2024).

Figure 1. Diagram of the process of producing biomass and oil from Parachlorella sp.

*Table 2. Stoichiometric reactions*

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Reaction | Equipment | Stoichiometric reactions |  |  |  |  |  |  |  |
| Biomass cultivation from Parachlorella sp. | Reactor 1 | 56.4CO2 + 1000H2 + 424O2 + 17.82NaHCO3 + 17.821NH4Cl → 74.22CH1.68O0.46N0.24 + 982H2O + 17.82NaCl (1) | | | | | | | |
| Formation of HCO3 from CO2 |  | 72CO2 + 72H2O → 72HCO3- + 72H+ (2) | | | | | | | |
| Carbon fixation (Calvin Cycle) |  | 72HCO₃⁻ + 72NADPH + 108ATP + 72H2O → 12C6H12O6 + 72H2O + 72ADP + 72Pi + 72NADP+ + 72O2  (3) | | | | | | | |
| Glycolysis and pyruvate pathway |  | 12C6H12O6 + 24H2O → 24C3H4O3 + 12ATP + 96NADH + 12O2 (4) | | | | | | | |
| Tricarboxylic acid cycle (Krebs cycle) |  | 24C3H4O3 + 24CoA + 2NAD+ → 24C2H3O−S−CoA + 24CO2 + 24NADH (5) | | | | | | | |
| Fatty acid synthesis (Acetyl-CoA carboxylase and fatty acid synthase pathway) |  | 24C2H3O−S−CoA + 42NADPH + 21ATP → 3C16H32O2 + 24CoA + 42NADP+ + 21ADP + 21Pi + 9H2O + 4,5O2  (6) | | | | | | | |
| Formation of C3H8O3 |  | 0,5C6H12O6 + ATP + 2NADH → C3H8O3 + ADP + Pi + 2NAD+  (7) | | | | | | | |
| Palmitate esterification (triglyceride synthesis) |  | 3C16H32O2 + C3H8O3 → C51H98O6 + 3H2O (8) | | | | | | | |
| Global reaction: Formation of tripalmitin oil from CO2 | Reactor 2 | 51CO2 + 117NADPH + 122,5ATP + C3H8O3 → 78H+ + C54H103O9 + 117NADP+ + 97ADP + 97Pi + 9H2O + 91,5O2 + 118NADH (9) | | | | | | | |

1. Results

*Parachlorella* sp. is a species of algae that belongs to the *Chlorella* family and is characterized by its high production of lipids, starch, proteins and carbohydrates in short periods of time (Singh & Sharma, 2012). They are photosynthetic and photoautotrophic microorganisms that use light as an energy source and inorganic carbon (CO2) as a carbon source (Mahmood et al., 2022), demonstrating a high potential to produce biofuels with higher performance and lower resource consumption (Abdelsalam et al., 2019; Escobedo & Calderón, 2021).

The reactions presented in Table 2 were considered but in their overall form in the biomass reactor and oil reactor (Figure 1). Similarly, the modeling of oil formation was treated as an independent reaction in a separate reactor, this phenomenon is related to the stress required to increase the oil concentration. It has been reported that nitrogen, oxygen, and phosphorus depletion can increase oil production in *Parachorella* sp. (Mahmood et al., 2022)

Table 4 shows the global mass balance for each stage in the production process. The primary energy consumption in this process is associated with the formation of biomass and oil. This is a key aspect, as the energy source is solar energy, making the process both cost-effective and low in CO₂ emissions. The centrifugation stage is the second most energy-consuming phase of the process (540.061 kW). This high energy requirement is due to the low density of the biomass (approximately 1.1 g/mL), which is near the water density. In industrial processes, it is common to add adsorbent substances to increase the density of the biomass and reduce the power required for its recovery. In the simulation, we assumed that no adsorbent was added. Therefore, the energy consumption could be lower than the reported value.

Similarly, extraction with hexane is not highly energy-consuming because of the low pressure used in the system (0.4 atm). Low pressure is very common in extraction for avoiding reactions at high temperatures, which could decrease the quality of the oil. The low temperature (70°C) and high pressure are sufficient for evaporating the hexane. The hexane loss rate was low (5.84 kg/h), so the extraction was very efficient.

*Table 3. Energy required by stages*

|  |  |  |  |
| --- | --- | --- | --- |
| Stage | Energy (kW) | Mass balance  Inlet flow (kg/hr) | Mass balance  Outlet flow (kg/hr) |
| Biomass formation | 27070.100 | 19636 | 19635 |
| Oil formation | 3434.920 | 1250 | 1250 |
| Centrifuge | 540.061 | 9808.59 | 9808.58 |
| Dryer | 7.376 | 561.80 | 561.79 |
| Hexane extraction | 0.001 | 604.90 | 604.90 |
| Recirculated hexane | 24.319 | 374.24 | 374.24 |
| Evaporator 2 | 7.534 | 243.83 | 243.83 |

*Table 4. Mass flows*

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | Stream flows (kg/hr) | | | | | |  |  |  |  |  |  |
| Components | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
| Biomass | 10 | 345.4 | 0 | 345.4 | 0 | 345.4 | 0 | 345.4 | 354.4 | 0 | 0 | 0 |
| Water | 1000 | 8127.2 | 0 | 7578.4 | 7575.1 | 3.3 | 194.3 | 0.1 | 0 | 0 | 0 | 0 |
| Carbon dioxide | 1000 | 0 | 625 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Oxygen | 13185 | 7718.9 | 813 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Hydrogen | 2000 | 1187.8 | 21 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Sodium bicarbonate | 605 | 1.9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Ammonium chloride | 385 | 0.9 | 0 | 0.9 | 0.7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Sodium chloride | 0 | 419.6 | 0 | 419.5 | 419.4 | 0.1 | 0 | 0 | 0 | 0 | 0 | 0 |
| Hexane | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 754.1 | 748.3 | 5.8 | 5.8 |
| Tripalmitin oil | 0 | 0 | 0 | 224.8 | 0 | 224.8 | 0 | 224.8 | 224.8 | 0 | 0 | 224.8 |

On the other hand, the process absorbs CO₂, contributing to atmospheric decarbonization. The production of biomass and oil from algae provides an important source of raw materials for third-generation biofuel production. The biomass yield from CO₂ is 0.336 kg of biomass per kg of CO₂, which is lower than some values reported in the literature (0.546--2 kg biomass per kg of CO₂) (Li et al., 2011). The oil yield is 0.346 kg of oil per kg of CO₂, and the oil content in the biomass is 66.82%, which is similar to that of some algal species (greater than 50%) (Jaiswal et al., 2022). Another important aspect of biomass formation is the production of oxygen (8531.93 kg/h), which positively impacts air quality.

This highlights the potential of algae as an excellent means of decarbonization, as they can capture up to five times more CO₂ per hectare than terrestrial crops, such as palm oil (Chanana et al., 2023). The use of algae-derived oil in biodiesel production results in a lower carbon footprint. Additionally, residual biomass can be converted into other biofuels through processes such as pyrolysis or gasification.

1. Conclusions

It is important to recognize that results may differ from reality due to multiple factors, such as environmental conditions, light intensity, temperature, nutrients (mainly nitrogen and phosphorus), pH, and salinity, which can vary in real-life environments and affect cell growth and lipid accumulation. Furthermore, differences between the mathematical models used in the simulation and the actual physiology of microalgae can introduce discrepancies. Operational factors, such as the efficiency of the cultivation systems and the presence of contaminants or biological competitors, can also influence the final results. Therefore, it is essential to validate the models with experimental data and consider these aspects when interpreting the simulation results. However, no proprietary experimental results were used in this simulation; all data used were obtained from the scientific literature. Previous studies that report relevant parameters for microalgae growth and lipid accumulation under different conditions were selected. This allowed us to build a model based on previously validated data, although it involves certain limitations, since the specific conditions of each study may differ from a controlled experimental environment or industrial applications.

In this work, the production of *Parachorella sp*. in a bioreactor was simulated. The flow of matter and energy was established. The process stages with the highest energy consumption are biomass and oil formation, both of which are powered by solar energy. In this way, a total of 1600 kg of CO₂ is consumed every 224.80 kg of oil produced. As a result, decarbonization of the atmosphere can be achieved while producing oil for third-generation biofuel production. The recirculation of hexane shows that nearly 5.84 kg/h is lost during the process. The integration of alternative energy sources into the process could help achieve a negative CO₂ balance, contributing to the decarbonization of the planet.

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