Sustainability Assessment in Chemical Processes

A case study in a Brazilian cosmetics industry

Julia Rocha de Moura Campos

Department of Engineering and Management, Instituto Superior Técnico, Universidade de Lisboa, Portugal

Abstract

This paper discusses sustainable development as the way to guarantee the human well-being and fight resource scarcity. It focuses on the Brazilian sustainability scenario and exposes the urgency of further development of governmental policies and the important role of companies for its progress. Life Cycle Analysis is presented as a method to quantify and compare environmental loads, applied in this study with software SimaPro.

The discussion on sustainable development unfolds to the analysis of sustainability in chemical processes. This paper presents and discusses a case study composed by two situations concerning the efficiency in the use of resources in a Brazilian cosmetics industry The first situation regards the discard of 550 liters of clean utility water after a batch cooling and the second case concerns to the reduction of one cooling task duration of the process.

Keywords: Sustainability, Improve Efficiency, LCA Analysis, Batch Processes

1. Introduction

Since the industrial revolution countries have developed their progress based on a mass consumption society, supplied by industries that exploit natural resources and fossil fuel energy. This major shift in human kind history brought great benefits for the society, but at the cost of earth exploitation. Climate change, resource scarcity and other threats lead to the discussion of sustainable development and how to achieve it.

The first world conference about the environment was held in Stockholm in 1972 and since then nations have been discussing sustainable alternatives of progress that attend the established goals. Although the discussion evolved in terms of content and complexity, sustainability continues to be an abstract concept that depends on the interpretation. Thus, an initial step in a sustainable development study is defining its definition and scope.

The most common interpretation of the concept and the one in which the study is based on is from the 1987 World Commission on Environmental Development, which states, "Sustainability development is development that meets the needs of the present without compromising the ability of future generations to meet their own needs". Furthermore, the scope of the present study is to analyse sustainable development in a cosmetic industry and discuss it under the environmental and economic pillars.

2. The importance of promoting sustainability in Brazil

As well as in European countries, sustainable development is seen in Brazil as the alternative to the environmental, social and economic problems faced by the current generation. Although sustainability is the subject of many actions and debates, the country is clearly behind when compared to goals set in world conferences and by European organizations.

Brazilian ecosystem holds the world's greatest diversity, setting the country to number one among the 17 most biodiverse nations. Besides natural heritage, Brazilian biodiversity has a central role in the national economy. The agroindustry sector alone is responsible for 40% of the Gross Domestic Product; the products that derives from biodiversity stands for 31% of all exportations; and one third of all energy generated in the country comes from plant biomass (2).

The Brazilian Institute of Geography and Statistics (*Instituto Brasileiro de Geografia e Estatística, IBGE*) developed a research in an attempt to evaluate holistically the progress of sustainable development in the country. Entitled "Population, Space and Sustainability – Contributions to the development of Brazil" (*"População, Espaço e Sustentabilidade - Contribuições para o desenvolvimento do Brasil"*), the study carried in 2011 measures the performance of different sectors under the perspectives of 'human well-being' and 'ecologic well-being'. Results show that Brazil had little progress towards a more sustainable development and is on the verge of unsustainability. There have been some advances in relation to human well-being, but very few in relation to ecological well-being. Far from a sustainable development, the country had the worst results when the subjects were ocean protection, biodiversity and basic sanitation service. The socioeconomic analysis of both years exhibit production and consumption models potentially unsustainable.

2.1. The role of Brazilian companies in achieving sustainable development

On the other hand, sustainability is a present issue in the business sector, which shows more concern on the subject. According to a study, 69% of the companies in Brazil recognize the need to include sustainability in the strategic planning (3). The main topics related to sustainability in the private sector are: innovation, risk, impact in the value chain, business opportunities and social inclusion.

The Brazilian companies follow the same pace of the international market, which starts to realize the value of sustainability for the business. A MIT research carried out between 2011 and 2012 shows that one third of the interviewed companies from more than 100 different countries recognizes that sustainability contributes to increase profits. In addition, sustainability showed to be correlated to business resilience, since a great number of companies enlarged their investments in sustainability during the economic crisis of 2008 and 2010 (4).

Although sustainability is present in the Brazilian private sector, there is a lot to progress. There are few Brazilian companies that can be considered sustainability leaders, which means that they have a consistent strategy to face the complexity of the issue. However, the ones that are considered leaders, are at the same level of their international peers. The progress achieved so far is not enough to create a new economy that guarantees the sustainable use of natural resources and the improvement of the quality of life. Nonetheless, this progress already reveals the importance and potential of the business sector for the sustainable development in the country.

3. A tool to measure sustainability: Life Cycle Analysis

Now-a-days is essential for companies' processes decision-makers to include Sustainability actions, however for that it is crucial to quantify its effects. Since the end of the 20th century, many tools to assess sustainability have been designed, some examples are: Life Cycle Costing (LCC), Life Cycle Analysis (LCA) and risk assessments. Because this type of assessments involves uncertainties and abstract terms, they have to be carefully applied and always considered alongside an interpretation of the methodology used.

Among all available environmental methodologies, European Commission considered LCA the best tool to assess the life cycle impacts of products (5). Therefore, the present paper further investigates the advantages and limitation of the LCA methodology and SimaPro as a software and applies it in an industrial case study.

According to ISO 14040 report (6) life cycle assessment is the "compilation and evaluation of the inputs, outputs and the potential environmental impacts of a product system throughout its life cycle". ISO also defined the tool as a comprehensive assessment that considers all aspects of natural environment, human health and resources.

What differs LCA method from other environmental assessment tools are: the life cycle approach and the focused analysis on the product's function, rather than unit (7).The "cradle-to-grave" assessment allows a proper comparison among alternatives, since it avoids problem-shifting. Products have different impacts on the environment in the different life stages, considering the whole framework prevents a biased interpretation, since the results vary according to the phases considered. The same problem could happen when favouring a region or an impact category over another.

LCA has two major applications: as a decision support tool and in the evaluation of the environmental load. The first application is convenient in the case of comparing different alternatives regarding their impacts or studying improvements in the efficiency of a system in terms of energy and material deployment. As for the second application, an example is the identification of dominant environmental problems regarding a good.

The methodology is composed of four steps: goal and scope definition, life cycle inventory analysis (LCI), life cycle impact assessment (LCIA) and interpretation.

3.1. Limitations of the method

Regarding limitations of the method, Life Cycle Analysis encounters limitations common to environmental assessment tools and limitations specific to the methodology.

The main limitations shared by all environmental tools, including LCA are: the analysis is circumscribed to the boundaries chosen in the scope definition of the study; there are uncertainties due to the difficulty in modelling the complexity of the real world; there are inaccuracies in data that comes from measurements' imperfections, systematic errors or unrepresentative data used to cover gasps (8).

On the hand, the primary category-specific limitations on the accuracy of the LCA framework, are: LCA high dependence on data, which makes the results questionable in cases of gasps or inaccuracy (9); the fact that the results can only be interpreted in association to the goal and scope of the analysis, which reflects the stakeholders' point of view; the loss of temporal and spatial characteristics due to simplification in the model as, for example, aggregation; the divergence in existent methods to assess impacts and normalization factors; the lack of a methodology allow the use of the methodology to endorse personal interests (10).

3.2. SimaPro software

SimaPro is a modeling and evaluation program launched in 1990 by the group PRé Consultants that allows the design, analysis and monitoring of the sustainability profile of products and services (11). It makes it possible to evaluate complex life cycles in a systematic and transparent way through simple modeling. Therefore, the program includes an interface for life cycle modeling, a process and impact assessment database, that comprises several methodologies, and a calculator that computes the values withdrawn from the database and the designed model (12).

The SimaPro user follows the step by step of the LCA methodology: introduction of the ambit and scope of the project, modeling of the processes involved in the study and evaluation of the systems according to the different impact categories of the initially selected methodology.

The modeling process is performed systematically and has the support of an extensive database, that can be edited by the user. SimaPro makes it possible to model several scenarios of materials disposal and associate them with the processes to which they are applied. The results are displayed as an extensive inventory table or in the form of a diagram, which makes it easier to visualize.

There are many functions available to analyze the results in SimaPro, such as characterization, parameters for sensitivity analysis and graphs to compare two life cycles.

A great advantage of this software the versatility: the basic tools simplicity allows users without experience to understand the program, while the wide range of functions and tools enables the modeling of more complex systems and deeper analysis. The only disadvantage of the software is its high cost, which despite being compatible with the market, makes it hardly accessible for everyone.

An aspect for improvement is the lifecycle modeling interface, which instead of an extensive listing of processes and materials, could have a graphic display to facilitate the search.

4. Case study in a Brazilian cosmetics industry

The company in which the case study takes place is a multinational Brazilian company of the beauty and personal hygiene sector, whose commitment is to develop products that express sustainable values and behaviours. They are a B Corporation, which means that they give equal value to their economic and socio-environmental results. Because they are constantly searching new ways to improve operations efficiency and sustainability, the company suggested the study of two situations currently faced by one of their manufacture units in Brazil.

The operations in the factory under study occur as a batch system in 8 reactors that, after mixing the product, go under a cool down process. The cooling fluid is water at 8ºC and the total duration of the heat exchange is 60 minutes. After the process is finished, the water left inside the reactor's jacket is purged with compressed air at 6 bar and discarded together with other effluents from the process. This routine happens, approximately, 3 times a day and the factory operates 6 days a week.

There are two study trends: the discard of cold water and the long duration of the cool down process.

4.1. Subcase A: The discard of cold water

The decision of discarding the cold water and not reinserting it back into the cooling system is the right action to guarantee the process safety. The mixed air in the water increases the corrosive nature of the fluid and deteriorates pipes and equipment. The corrosion is driven by the oxygen and accelerated by acid substances like carbon dioxide, sulphur dioxide and other gases that are found in the air. Oxygen is a highly reactive substance, especially in the presence of water. Its oxidation potential triggers a reaction with metals, removing their electrons and forming oxides as by-products.

Therefore, it is imperative to treat the water before reinserting in the cooling system. Currently, the discarded water joins the effluent stream and proceed to a physical-chemical treatment in an external effluent treatment station. However, the aired-water doesn't require such a complex treatment and, eventually, enlarges the effluent stream, spending unnecessary resources.

4.1.1. Solution design

The suggested solution is to add a treatment unit inside the factory that removes the air present in the water. This separation process is called deaeration, which is a particular method of desorption.

Desorption is the opposite of absorption and consists of the removal of gaseous components from the solvent through mass transfer (13). There are several practical methods that depend on the complexity and purpose of the application, but all work on the principle that the gas solubility in the liquid decreases with increasing temperature and pressure drop. The most common equipment are: plate, spray and packed columns.

As it is a quiet simple application and there aren't enough data to support the design of a complex equipment, the solution is a single plate column and it is designed based in the theoretical principles of deaeration.

The deaeration process is instantaneous, thus, it is can be designed as a continuous process. However, it should follow the batch dynamic of the cooling processes, which discard in the end 550 litres of aired-water. Hence, the deaeration process should work as semibatch unit of $0.55m^3$.

The lowest pressure obtained without the use of compressors is the atmospheric pressure. The of oxygen solubility in water with 3 ppm of chlorine at atmospheric pressure is given in table 1.

Table 1. Oxygen solubility in water at atmospheric pressure with 3 ppm of chlorine at different temperatures

Oxygen solubility in water with 3 ppm of Chlorine			
42ºC	6.05 mg/L	**45ºC**	5.77 mg/L
43ºC	5.95 mg/L	**46ºC**	5.69 mg/L
44ºC	5.86 mg/L	**47ºC**	5.59 mg/L

The concentration of oxygen in the cold water used in the industry is 6 mg/L, therefore, the temperature reached in the deaerator must be higher than 43ºC. Including a safety margin, the suggestion is a deaeration process at 45ºC

Since the volume of water treated per batch is relatively small, it can be used a plate heat exchanger to rise the temperature of the water. The equipment area is calculated through the heat exchanger equation.

$$Q' = UA\Delta T_{LMTD} \qquad \text{(eq. 2)}$$

The global coefficient is taken from the literature for carbon steel pipes, $U = 1050\, W/m^2K$ (14). The ΔT_{LMTD} is calculated from the steam temperature (120.2ºC) and the inlet and outlet temperatures of the water (10 and 45ºC). The energy flow is based on the amount of energy needed to heat the water, calculated from the following formula:

$$Q' = M'Cp\Delta T \qquad \text{(eq. 3)}$$

Where M' is the mass flow, adopted as $1.39\ kg/s$. The result is a heat exchanger with $A = 2.1\ m^2$.

The treatment system is composed of a 0.55 m^3 vessel, a plate heat exchanger with total contact area of 2.1 m^2 and a tank with an electric mixer device. All equipment must be made from stainless steel due to the corrosive potential of the water.

4.1.2. Life Cycle Analysis

The goal of the assessment is to compare the current treatment scenario for the aired-water (Current Alternative) with the deaeration solution proposed above (Subcase A Alternative). The **functional unit is the treatment for reuse of 550L of aired-water per batch**.

The considered lifespan of all equipment is 20 years. The connection pipes and the pumps are not included in the study. The LCA was performed with the software SimaPro and the method selected for the impact assessment was World *ReCiPe I/I, from ReCiPe Endpoint (I) version 1.13*.

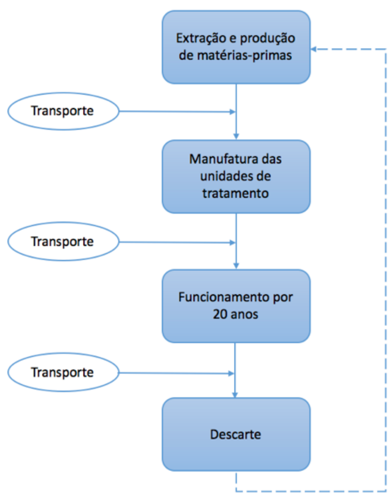

Figure 1. Scope considered in the modelling of the infrastructure of the water treatments compared

Before interpreting the results obtained is important to go over the uncertainties and limitations of the modelling. The main source of uncertainty of the LCA is the fact that SimaPro database is focused on European processes and the case study is in Brazil, thus, part of the data used is broad and doesn't reflect so well the specificities of the context. The second source of uncertainties is the hypothesis that all material and energy flow from the mass balance of the Current Alternative are proportional to the volume of aired-water that goes to treatment. Furthermore, some resources use, like pipes and pumps, were left out of the model.

Table 2. LCA Single score results using SimaPro

Global Score	Pts
Subcase A Alternative	1.15
Current Alternative	1.58

In terms of single score given in points (Pts) in table 2, the deaeration treatment shows to be 27% less impactful than the effluent treatment. The next step is to analyse the options under the impact categories available.

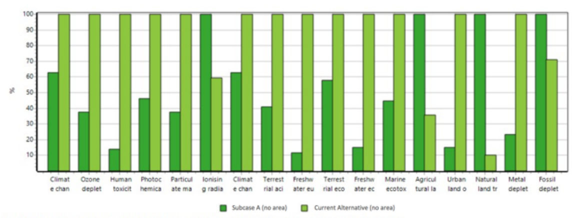

Figure 2. comparison of Subcase A Alternative and the Current Alternative performances in the impact categories (figure from the software SimaPro)

In the 17 impact categories (Figure 2), the deaerator appears to be more environmentally friendly than the effluent treatment station in 12 of them. The exceptions are: fossil fuel depletion, natural land transformation, agricultural land occupation and ionic radiation. From the process contribution analysis, the steam use is the main process contributing to fossil fuel depletion and ionic radiation and the electricity use the main factor contributing to natural land transformation and the occupation of agricultural land.

A future study development of the deaeration solution can be the replacement of steam for other heating sources or the use of vacuum in the deaeration. The score of the electricity use can be diminished with the study of the minimum time period the mixer needs to work in the deaeration process.

On the other hand, from the process contribution analysis of the Current Alternative, the use of chemical products and the discard of the physical-chemical sludge are, together, the most harmful aspects of the effluent treatment.

4.1.3. Financial Assessment

The financial calculations include investment and operation costs. The investment cost comprises the price and installation cost of each equipment. The last parcel is usually approximated as the equipment market value. The operational cost should consider resources use and maintenance cost. However, for this study, the maintenance costs are disregarded since they are small values when compared to the resource consumption. The costs are displayed in table 3.

Table 3. Investment costs

	Market Price ($)	Price with Installation ($)
Tank	486[1]	972
Heat exchanger	1458[2]	2916
Electric mixer	1080[3]	2160
Total		6048

The resources consumed in the operation is basically composed of the steam from the heat exchange process. The deaeration process required 36.1kg of saturated steam at 120.2ºC to heat the water 35 degrees Celsius. The fuel burnt in the industry to produce the steam is ethanol, which costs $ 0.65 and generates 7 kilograms of steam per 1 litre of alcohol. The calculations result in a cost of $ 3.37.

[1] Information given by Passafaro company

[2] Information given by Bermo company

[3] Information given by Bomax company

The following step is to compare it with the operations cost of the effluent treatment station.

The current alternative spends $ 5.30 to treat 550L of industrial effluent. However, considering the 33% efficiency of the treatment system, the price to treat and make the water ready for reuse is $ 8.84. Thus, the total savings per batch are $ 5.47

Dividing the investment cost and considering 3 batches per day, 6 days per week, the discounted payback period of the investment is 16 months.

4.1.4. Sustainability Analysis

The tools applied in both analysis show that the implementation of the solution designed in this case study is a decision towards a more sustainable process. The assessments indicate that the disposal of the aired-water is more expensive to the industry, giving that in only 16 months from the implementation the industry will save $ 5.47 per batch. In addition, it is a more harmful choice to the environment, since the solution proposed outperformed the current treatment option in 13 out of the 17 criteria and also in global terms.

The LCA showed that the main problem of the effluent treatment system is that it applies chemical treatment when it is not needed. On the other hand, the analysis also allows to identify improvements in the solution designed in order to further develop the alternative. Future developments should study more environmentally efficient alternatives to the saturated steam and the electric mixer.

Finally, to conclude the sustainability analysis, the process safety is discussed. Overall, the fact that the deaeration process is an exclusively physical treatment, makes it a safer alternative to the employees and the industry. However, the effluent treatment station is a well stablished process and the deaeration system requires regular maintenance planning. In addition to that, it is important to control de quality of the deaerated water, especially in terms of acidity, because the corrosion of pipes and equipment jeopardize the whole process safety.

4.2. Subcase B: The long duration of the process

The second study aspect is the possibility of reducing the duration of the cooling process in the reactor, in order to reduce overall process time. This study reflects on the availability of the equipment, which have significant impacts in the industry.

There are several ways to increase heat exchange in a cooling process: increase the contact area, change equipment's material, increase the pressure difference in the cooling fluid side or change its nature. The first two alternatives require changes to the reactors of the factory, which makes them unfeasible.

The factory's cooling system is made in conjunction with the office cooling, which restricts the temperature of the cold water to above zero degrees Celsius. Therefore, replacing the water for another cooling fluid is not a good option, since studies demonstrate the superiority of the cold water as cooling fluid for temperatures above zero degrees Celsius (15). Likewise, the option of increasing the pressure difference is not a responsible approach, since the site engineers mentioned that the system faces a pressure drop problem due to pipe clogging. The option that remains is to study the influence of the cold water inlet temperature in the process duration.

4.2.1. The influence of the temperature in the process duration

The lack of data of the heating process requires some estimations on the model. First it is assumed that the product inside the reactor vessel is perfectly mixed and that the heat exchange process is adiabatic. Then, the heating profile of the cold water is considered constant in time and with fixed variation in space. The outlet temperature of the jacket is set to an average value of 10ºC.

Knowing that the inlet and outlet temperatures of the mix inside the reactor vessel is 80 and 35ºC, respectively, and knowing that the cold water flow is 16 m^3/h, it is possible to reach the equation 4 that models the heating process. The model is the sum of the heat exchanger and the heat amount equations (eq. 2 and eq. 3).

$$Q'[MJ] = 2{,}93\Delta T_{LMTD} \quad \text{(eq. 4)}$$

Table 4. New process durations for lower inlet temperatures of the cold water

T inlet	Q' (MJ/h)	Cooling duration (min)	Reduction in time (%)
7ºC	134.3	59.08	2%
6ºC	136.3	58.21	3%
5ºC	138.3	57.37	4%
4ºC	140.3	56.56	6%

4.2.2. Financial assessment

On one side of the financial analysis there are the extra expenses with electric energy to cool down the cold water stream and, on the other hand, the gains with the increase on the factory productivity. To facilitate the analysis, it is considered that when a reactor is made available, it will be used to make more product.

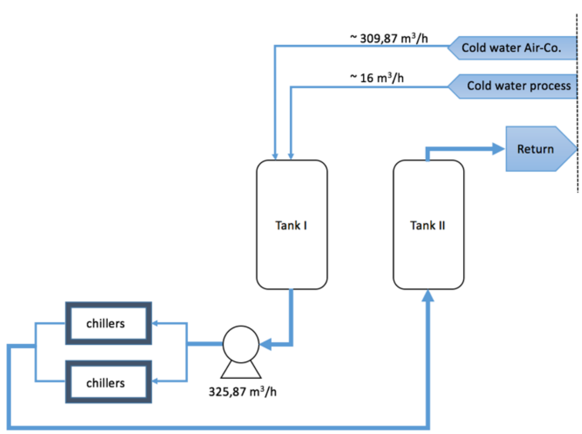

Figure 3. Cooling system that serves the factory and the air-conditioning equipment

The required energy flows ($Q'_{T=Ti}$) to cool down the water streams are found replacing the flows from figure 5 in the equation 3. With the estimated functioning hours of the chillers (H_C) and the price of the industrial electric power, 89.189 $/MWh, it is possible to calculate the monthly cost of keeping the cold water in lower temperatures.

$$Cost_{T=Ti} = 330.33\ x \sum Q'_{T=Ti} . H_C \quad \text{(eq. 5)}$$

Table 5. Extra energy required and equivalent costs to keep the cold water at lower temperatures

T inlet	Extra energy consumed per month	Monthly cost
7ºC	44.6 MWh	$ 3,975.21
6ºC	89.1 MWh	$ 7,950.69
5ºC	133.7 MWh	$ 11,925.90
4ºC	178.3 MWh	$ 15,901.38

The following step is to estimate the gains from the extra production. The process is working on average 3 times a day and produces in 1 hour eight tons of product per reactor. To transform it into a comparable value, the yield is divided by the costs, calculating a minimum net profit margin per extra litre produced.

Table 6. Extra earnings and minimum profit margin per litre of product

T inlet	Extra production (ton./month)	Minimum net profit margin (BR$/L)
7ºC	8.8	0.45
6ºC	17.2	0.46
5ºC	25.3	0.47
4ºC	33.0	0.48

It is possible to go further in the analysis in order to produce more decision support tools and assess different sales scenarios. Based on a positive scenario of sales corresponding to 100% of the extra volume produced, the profitability of the project can be calculated as a function of the net profit margin. Profitability (L) is calculated from the actual net profit margin (MLR), the extra production (P_{extra}) and the cost of production per litre ($C_{prod/L}$):

$$L = (\%sales\ x\ P_{extra}\ x\ MLR) - (C_{prod/L}\ x\ P_{extra}) \quad \text{(eq. 6)}$$

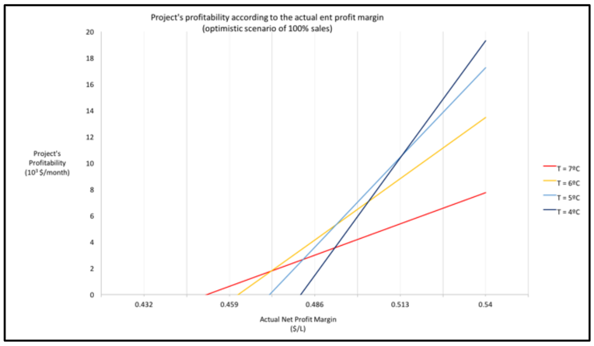

Figure 4. Project profitability as a function of the actual net profit margin for different temperatures

With a net profit margin per litre of product greater than $ 0.45, profits from the extra production outweigh the costs of cooling the water and the implementation of the project is financially sustainable. In the best of the scenarios, which considers total sale, with a net profit margin of 0.49 $/L, reducing the temperature in 2 ºC yields $ 4,050.00 per month.

4.2.3. Sustainability Analysis

Because LCA is not an appropriate tool to assess the project and it is difficult to quantify the gains from the equipment availability, the environmental assessment is developed in the form of a cost-benefit discussion. On the one hand, the solution of reducing the water temperature requires higher power from the chillers, spending more energy, as calculated in table 9 of the financial analysis. On the other, it reduces the operating time of the reactor, the electric mixer and the pumps that feed the jacket with cold water.

Regardless of the energy balance, the separation of the cooling systems is essential to increase process efficiency, flexibility and to reduce both environmental and financial impacts.

The study shows that it is possible to achieve a monthly profit of $4,050.00, which result in annual profits of $ 48,600.00.

For a future development of the study, it is suggested to investigate possible cold streams available in the process that could decrease the need for external cooling sources. Also, analyse the effects of adding cold water directly in the mixture inside the reactor, since water is one of the ingredients that composes the product. This greatly increases the efficiency of the heat exchange, but may have consequences in the texture or quality of the product.

5. Conclusion

The world suffers from the results of a society that has been created around a linear economic model driven by consumption. Sustainable development is the key answer to environmental problems faced nowadays.

However, house for the greatest biodiversity on the planet, Brazil presents ecological and human well-being indexes that border unsustainability and evidence the urgency of this subject for the country. The Brazilian industry starts to recognize the importance of sustainability and include it in their business strategies. In this context, Life Cycle Analysis can be a powerful tool to compare the sustainability of alternatives and support future changes.

The industry case studies approached regard improvements in the efficiency of resources use. The solution proposed in the first subcase A is the insertion of a deaeration system which allows the reincorporation of the water in the cooling system. In the second, it was suggested to decrease the inlet temperature of the cold water in the reactor jacket.

The solution for the subcase A demonstrated to be a profitable project, with a payback period of 16 months. With a global score 27% lower than the current disposal scenario in the LCA, the deaeration proves to be an alternative with less environmental impacts, especially because it is an exclusively physical water treatment.

In the subcase B, the simulation of the heating process with reduced temperatures created the possibility of many profitable scenarios. For a net profit margin of 0.49 $/L, reducing the temperature in 2 ºC yields $ 48,600.00 of extra profits per year.

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