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Life Cycle Analysis of Dye Degradation Using Advanced Oxidative Processes

Rogério F. Silva[a], José V. S. Aragão[b], Pedro H. D. Matos[b], Victória F. A. Milanez[a], Jacqueline S. Macêdo[c], Armando D. Duarte[b], Osmar V. Araújo[b], Gilson L. Silva[b], Andréa F. S. Costa[b]*

[a]Campus Belo Jardim, Federal Institute of Education, Science and Technology of Pernambuco, Avenue Sebastião Rodrigues da Costa, no number, São Pedro, zip Code: 55155-730, Belo Jardim, Pernambuco, Brazil.
[b]Agreste Region Academic Centre, Federal University of Pernambuco, Campina Grande Avenue, s/n, Nova Caruaru, Zip Code: 50670-90, Caruaru, Pernambuco, Brazil.
[c]PRODEMA, Federal University of Pernambuco, Cidade Universitária, s/n, zip code: 50740-540, Recife, Brazil.
andreafscosta@hotmail.com

Pollution caused by textile processes has led several countries to create stricter environmental legislation for the treatment of industrial effluents. Since, to meet legal requirements, the degradation of these chemical dyes must have a low environmental impact and high removal efficiency.
This study performed the Life Cycle Analysis (LCA) of the degradation of dyes in 1 m³ of effluent, through advanced oxidative processes, using the Photo-Fenton process. For the Life Cycle Inventory (ICV), the compounds Hydrogen Peroxide (H_2O_2) and Iron (II) Sulphate ($FeSO_4$) were considered. The methodology for calculating environmental impacts was ReCiPe 2016 Midpoint (I) V1.04 / World (2010) I and the impact categories of the studies were: Global Warming, Freshwater Eutrophication, Freshwater Ecotoxicity and Human Carcinogenic Toxicity. The sensitivity analysis occurred in comparison with the methodologies: IPCC 2013 GWP 20a V1.03 and CML-IA baseline V3.06 / World 2000. All simulations occurred in the SimaPro® software, Faculty version, and pointed to H_2O_2 as an important contributing agent, along with the secondary products formed by the degradation of the dyes by the Photo-Fenton process, for the environmental impacts of this treatment.
Keywords: Life Cycle Analysis, Dye Degradation, Photo-Fenton Process

1. Introduction

1.1 Advanced Oxidative Processes

Advanced oxidative processes are based on the release of free radicals, especially hydroxyl radicals (-OH), which are highly oxidative. Given the right circumstances, the degradation of chemical substances can occur quite efficiently. According to Tiburtius, Peralta-Zamora and Leal (2004), the hydroxyl radical can react with many organic compounds in different ways, could be by adding the double bond or by abstraction of the hydrogen atom in aliphatic organic molecules. According to Safarzadeh-Amiri, Bolton and Cater (1997), the results of these reactions is the organic formation of radicals that react with oxygen, thus initiating a series of degradation reactions, which can result in innocuous species, such as CO_2 and H_2O. These processes can be a very viable alternative to the treatment of effluents, as it is faster and requires fewer financial resources.
The advantages of advanced oxidative processes are that they open possibilities to degrade substrates of all chemical nature. One of its potential are degradation pollutants with low concentration or even the absence of waste generated.

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Studies in this area, such as the efficient technologies in the degradation of pollutants present in effluents and wastewater, have become an area of extensive investigation. Therefore, it is interesting to compare the results obtained in the laboratory along the effective application of these processes in the Chemical Industry.
According to Pignatello, Oliveros and MacKay (2006), Advanced Oxidative Processes are characterized by transforming, partially or totally, pollutants into simpler species such as carbon dioxide, water, inorganic anions or less toxic substances that can be degraded by common technologies. However, in some cases the degradation products of Advanced Oxidative Processes may be more harmful to the environment and less biodegradable compared to the original compounds.

1.2 Life Cycle Analysis

The NBR ISO 14040 and NBR ISO 14044, present and standardize an important tool to identify and assess environmental impacts. The current technical standard Abnt (2009a), presents 4 phases for structuring the life cycle analysis, which are: Definition of Objective and Scope, Inventory Analysis, Impact Assessment and Interpretation. Thus, it is possible to analyse from the extraction, manufacturing and final destination of natural resources throughout the product or service life cycle. For carrying out LCA studies, Duarte and Silva (2020) explain that it is important to delimit the boundaries of the analysed system, as there are several factors that can influence it. The boundaries exist to enable the problems to be solved, given the immensity of data that make up the analysed system (ABNT, 2009b). It can be characterized as the interface between a product / services system and the environment or other product / services systems (ABNT, 2009a). Therefore, the selection of data inputs and outputs must be consistent with the objective of the study. By understanding the need to assess the environmental impacts caused by advanced oxidative processes in the degradation of dyes, the life cycle analysis tool is very effective for this study.
According to Mata et al (2012) and Piemonte, Di Paola and Russo (2014), with that information in mind it is possible to identify workable solutions to the harmful effects on the environment. In this sense, this study sought to identify the effects of the treatment of degradation of dyes, from 1 m³ of effluent, through the Photo-Fenton process, using Hydrogen Peroxide as an oxidizing agent and Iron (II) Sulphate as a catalyst, in order to evaluate the possible impacts on nature resulting from this process. In addition to carrying out the sensitivity analysis of other calculation methods in LCA later.

2. Methodology

2.1 Structuring

The procedures for the treatment of industrial effluents aimed the removal of dyes effluent generated in the dyeing processes. The effluent collection took place in an industrial laundry on a textile pole, located in the Northeast region of Brazil. Standing out nationally for the manufacture of jeans garments.
The adopted methodology followed the Abnt (2009a), Abnt (2009b) and Silva (2015), where the ICV inputs were 15 kg of hydrogen peroxide (H_2O_2) and 5 g of iron (II) sulphate ($FeSO_4$), used in the treatment of the effluent. Silva (2015) performed the Photo-Fenton process with artificial light and sunlight and found different values of mineralization and reduction of Chemical Oxygen Demand (COD), which are shown in Table 1:

Table 1: Mineralization and COD reduction with artificial light and sunlight

Indicators	Artificial light	Sun light
Mineralization	41 % - 74 %	94.12 %
COD reduction	73 %	86.30 %

Since the process with sunlight discoloured the effluent, presenting greater mineralization of the dye and greater reduction of DOC, it was chosen . Therefore, it was not necessary to add electrical energy to the ICV, as the light used in the Photo-Fenton process came from solar radiation.
The functional unit adopted was 1 m³ of effluent and the reference flow was the treatment of 1 m³ of effluent with dye residues, resulting from textile processes.
For the validation of the Life Cycle Inventory (ICV), the levels of uncertainties were calculated through the Pedigree Matrix (SILVA et al. 2017 and TSAMBE et al, 2018). Performing the simulation in the SimaPro® software, Faculty Version, the significance of the potential environmental impacts from the ICV was assessed.

The results were interpreted based on specific impact indicators. In which the analysis method chosen was the ReCiPe 2016 Midpoint (I) V1.04 / World (2010) I, as it manages to rank the analysed impacts (ARAGÃO et al, 2020). The impact categories chosen were Global Warming, to analyse the emissions of carbon dioxide (CO2) to the atmosphere; Freshwater Eutrophication, to assess the potential effects of the release of this effluent on eutrophication in aquatic biota; Freshwater Ecotoxicity, selected to assess the toxicity of the release of this treated effluent into aquatic life; and Human Carcinogenic Toxicity, to assess harmful effects on human health. The results were interpreted based on specific environmental impact indicators.

2.2 Statistic

The analysis of the uncertainties of the data were performed through the inputs and outputs of the system. Abnt (2009b) states that in L.C.A. studies, the level of confidence in the data must be taken into account. Since possible variations may occur, techniques such as the Uncertainty Analysis and Sensitivity Analysis contribute to make the study robust and to make its results loyal to reality with a certain level of confidence.
The Analysis of Uncertainties evaluated the data obtained with 95 % confidence through the Pedigree Matrix (WEIDEMA and WESNAES, 1996). The 6 quality indicators and their levels of uncertainty were: Reliability (1.05), Completeness (1.05), Temporal Correlation (1.1), Geographical Correlation (1.01), Further Technological Correlation (1), Number of Samples (1.05) (ALTHAUS et al, 2004). The Basic Uncertainty Factor was 1.5 (PRÉ CONSULTANTS, 2016). The confidence level equation - Pedigree Matrix (Eq 1) was used for the calculation (BENEDET JÚNIOR, 2007):

$$SD_{g95} = e^{\sqrt{[\ln(U1)]^2 + [\ln(U2)]^2 + [\ln(U3)]^2 + [\ln(U4)]^2 + [\ln(U5)]^2 + [\ln(U6)]^2 + [\ln(Ub)]^2}} \quad (1)$$

Where:

- U1 = Uncertainty factor of the Confidence in the Source indicator.
- U2 = Uncertainty factor of the Completeness indicator.
- U3 = Uncertainty factor for the Number of Samples indicator.
- U4 = Uncertainty factor of the Time Correlation indicator.
- U5 = Uncertainty factor of the Geographic Correlation indicator.
- U6 = Uncertainty factor of the Technological Correlation indicator.
- Ub = Basic uncertainty factor.

In the sensitivity analysis, impacts were calculated using two different methodologies. The IPCC 2013 GWP 20a V1.03 calculation methodology considers global data, so that its simulation occurs more similarly to the global reality and not to a specific region. The CML-IA baseline V3.06 / World 2000, on the other hand, does not consider global data, so the simulation occurs more similarly to the European reality. For comparison the different categories of the ReCiPe 2016 Midpoint (I) V1.04 / World (2010) I methodology, the Global Warming category was chosen, as it is common to the three calculation methods.

3. Results

3.1 Simulation

The simulation results in Figure 1 presented themselves as expected in the inventory analysis, where hydrogen peroxide causes the main impact. In all categories, it presents percentages in the contribution of impacts greater than 99 %, as shown in Table 2:

Table 2: Emissions from Hydrogen Peroxide and Iron (II) Sulphate in the impact categories

Impact category	Unity	Total	Hydrogen Peroxide	Iron(II) Sulphate
Global warming	Kg CO_2 eq	25.60004	25.59887	0.00117
Freshwater eutrophication	Kg P eq	0.000634	0.000633	4.39E-08
Freshwater ecotoxicity	Kg 1.4-DCB	0.0113754	0.013753	5.6E-07
Human carcinogenic toxicity	Kg 1.4-DCB	0.010238	0.010238	1.5E-07

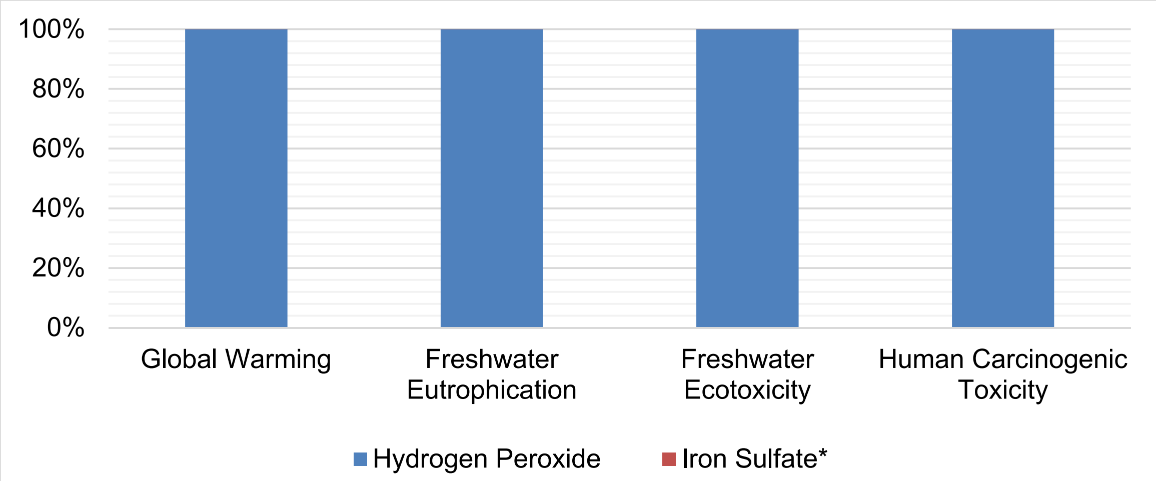

*Figure 1: Contribution of Hydrogen Peroxide and Iron (II) Sulphate in the impact categories. *The contributions of Iron (II) Sulphate were so irrelevant, that they could not be shown in this graph*

3.2 Analysis of Uncertainties

The standard deviation found in the Pedigree matrix was approximately 1.53 for the two process entries. In other words, the data show an uncertainty of 53 % (Table 3). According to Pré Consultants (2016), these high values occur due to the Basic Uncertainty Factor of the database, since they are prepared by specialists from different parts of the world, with data specific to their study locations. The confidence levels in the data collected through the laboratory redox process showed uncertainties that were much less than Basic Uncertainty Factor, with a maximum variation of 10 % in the Time Correlation dimension (U3).

Table 3: Attribute value in the Pedigree matrix

Dimension	Initials	Hydrogen Peroxide	Iron (II) Sulphate
Reliability	U1	1.05	1.05
Completeness	U2	1.05	1.05
Temporal Correlation	U3	1.1	1.1
Geographical Correlation	U4	1.01	1.01
Further Technological Correlation	U5	1	1
Number of Samples	U6	1.05	1.05
Basic Uncertainty Factor	Ub	1.5	1.5
Standard Deviation	SD	1.529773	1.529773

3.3 Sensitivity Analysis

The comparison of methodologies showed differences between the results. These differences are related to the geographic area covered by the methodology. Despite these differences, Hydrogen Peroxide continues to have the highest values in the Global Warming category.

3.4 IPCC

The results in Table 4 show practically identical results in the two calculation methods. Numbers that agree with Medeiros, Durante and Callejas (2018).

Table 4: Comparison between IPCC and ReCipe methodologies in the Global Warming category

Methodology	Unity	Total	Hydrogen Peroxide	Iron (II) Sulphate
IPCC	Kg CO_2 eq	25.57841	25.57724	0.00177
ReCipe	Kg CO_2 eq	25.60004	25.59887	0.00117

3.5 CML-IA

The result of the CML-IA method points to a reduction of approximately 20 % in relation to the ReCipe Midpoint (Table 5). Despite this difference, Pré Consultants (2016) states that these variations may occur due to data uncertainty. The contribution percentages remain practically unchanged, where H_2O_2 continues to present approximately 99 % contribution in the Global Warming category.

Table 5: Comparison between CML-IA and ReCipe methodologies in the Global Warming category

Methodology	Unity	Total	Hydrogen Peroxide	Iron (II) Sulphate
CML-IA	Kg C_2O eq	20.29287	20.29184	0.001028
ReCipe	Kg C_2O eq	25.60004	25.59887	0.00117

4. Conclusion

The study pointed out a workable solution for dye degradation in textile industrial effluents. Although the contribution rates of Hydrogen Peroxide in environmental impacts are greater than 99 % in all impact categories analysed, this Photo-Fenton process has a high rate of degradation and uses sunlight, making its application viable to replication in industrial scale. However, for these treated effluents to be released into water bodies, toxicity tests need to be carried out, aiming to guarantee environmental quality and the preservation of aquatic life.

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References

Abnt, 2009a, NBR ISO 14040, Gestão ambiental-Avaliação do ciclo de vida-Princípios e estrutura. ABNT.

Abnt, 2009b, NBR ISO 14044, Gestão ambiental-Avaliação do ciclo de vida-Requisitos e orientações. ABNT.

Althaus, H., Doka, G., Dones, R., Heck, T., Hellweg, S., Hischier, R., Nemecek, T., Rebitzer, G., Spielmann, M., 2004, Ecoinvent Report Nº 1: Overview and Methodology. Swiss Centre for Life Cycle Inventories, Dübendorf.

Aragão, J. V. S., Costa, A. F. S., Silva, G. L., Silva, S. M., Macêdo, J. S., Galdino Junior, C. J. S., Milanez, V. F. A.; Sarubbo, L. A., 2020, Analysis of the Environmental Life Cycle of Bacterial Cellulose Production, Chemical Engineering Transactions, vol 79, 445-450.

Benedet Junior, G., 2007, Avaliação de incertezas em inventários do ciclo de vida, Masters Dissertation, Technological Centre of Federal University of Santa Catarina, Florianópolis, Brazil.

Duarte, A. D., Silva, G. L., 2020, Application of Life Cycle Analysis (LCA) tool in the treatment process of effluents in a laundry of jeans, Exacta, vol 18(2) 355-368.

Mata, T. M., Martins, A. A., Neto, B., Martins, M. L., Salcedo, R. L. R., Costa, C. A. V., 2012, LCA Tool for Sustainability Evaluations in the Pharmaceutical Industry, Chemical Engineering Transactions, vol 26, 261-266.

Medeiros, L. M., Durante, L. C., Callejas, I. J. A., 2018, Contribuição para a avaliação de ciclo de vida na quantificação de impactos ambientais de sistemas construtivos, Ambiente Construído, vol 18(2), 365-385.

Pré Consultants, 2016, Introduction to LCA with SimaPro, Califórnia.

Piemonte, V., Di Paola, L., Russo, V., 2014, An LCA Study on Feedstocks and Processes for Biofuels Production, Chemical Engineering Transactions, vol 37, 517-522.
Pignatello, J. J., Oliveros, E., MacKay, A., 2006, Advanced oxidation processes for organic contaminant destruction based on the Fenton reaction and related chemistry, Critical reviews in environmental science and technology, vol 36(1), 1-84.
Safarzadeh-Amiri, A., Bolton, J. R., Cater, S. R., 1997, Ferrioxalate-mediated photodegradation of organic pollutants in contaminated water, Water Research, vol 31(4), 787-798.
Silva, F. B., Yoshida, O. S., Arduin, R. H., Vinhal, L. D., Teixeira, C. E., Oliveira, L. A., 2017, Análise comparativa de procedimentos para a estimativa de incertezas em ACV: um estudo baseado na produção de blocos cerâmicos de alvenaria, Brazilian Institute of Information in Science and Technology, 63-77.
Silva, R. F., 2015, Degradação de corante de efluente têxtil por processo oxidativo avançado, Doctoral Thesis, Federal University of Pernambuco, Recife, Brazil.
Tiburtius, E. R. L., Peralta-Zamora, P., Leal, E. S., 2004, Contaminação de águas por BTXs e processos utilizados na remediação de sítios contaminados, Química Nova, São Paulo, vol 27(3), 441-446.
Tsambe, M. Z. A., Almeida, C. F., Ugaya, C. M. L., Cybis, L. F. A., 2018, Inventário de Ciclo de Vida de Óleos Lubrificantes Usados ou Contaminados na Região Sul do Brasil, Revista Latino-Americana em Avaliação do Ciclo de Vida, vol 2(2), 9-33.
Weidema, B. P., Wesnaes, M. S., 1996, Data Quality Management for Life Cycle Inventories - An Example of Using Data Quality Indicators, Journal of Cleaner Production, vol 4(3-4), 167-174.