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Prospective Study on Chemometric Methods for Water Classification

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Abstract

Chemometric methods are currently used very frequently in water analysis. The present work deals with a bibliographic search, considering the scientific and technological developments of the water classification methods, in the area of chemometrics, through the search for articles and patents in the main databases available for research. The prospecting was carried out in the interval of ten years (2010-2020). 126 documents were found in the Scopus database, using the words water quality AND chemometrics. Regarding patents, 764 documents were found in the Espacenet database, with 184 filings in Questel Orbit® software, of which 145 are Chinese, 08 are Japanese, 04 are from the United States and 01 from Brazil. Therefore, this study showed a broad scenario for investing, by both public and private authorities. Although Brazil has a considerable amount of scientific articles on the subject, the number of patents has yet to be increased.

Key-words: Water Quality, Prospection, Physical-chemical Parameters.

1. Introduction

Water is an essential element for the survival of living beings and is also important in maintaining human health and animal welfare. Therefore, it is a vital resource for all living organisms, in the form of pure water, in habitats for aquatic life, and also being water for various purposes such as agriculture, industry and daily human consumption (Chou et al., 2018.).

Overall, Brazil has a considerable amount of water. It is estimated that the country has about 12% of the planet's freshwater availability, but the natural distribution of this resource is not balanced. The North region, for example, concentrates approximately 80% of the amount of water available, but represents only 5% of the Brazilian population. The regions near the Atlantic Ocean have more than 45% of the population, but less than 3% of the country's water resources (Agência Nacional Das Águas E Saneamento Básico, 2020).

In Brazil, the laws dealing with the potability of water for human consumption and animal watering and with groundwater are: Ordinance No. 2914 of 2011, Ministry of Health (BRASIL, 2016a), Resolution (RDC) of the National Council of the Environment (Conama): No. 357, of 2005 (BRASIL, 2005), amended by Resolution 410/2009 (Brasil, 2009) and 430/2011 (BRASIL, 2016b) and CONAMA's RDC No. 396 of 2008 (Brasil, 2008) (Bortoli et al., 2018).

Thus, to prove the quality of the water, it is necessary to perform microbiological and physicochemical analyses to check for compliance with the standards established by the laws in force in the country (Celligoi, 1999). Physical-chemical parameters are primary indicators of water quality, and the imbalance of these indicators may point to compromised water and result in health complications. These physical-chemical parameters are: Electrical conductivity; Hydrogen Potential (pH); Electrical resistivity; Temperature (ºC); Dissolved solids content (TDS); and Turbidity, in addition to total hardness, related to calcium carbonate and chloride contents (Parron et al., 2011).

Given this amount of parameters to be analyzed in laboratories, associated with the increasing sophistication of instrumental techniques of chemical analysis, which generate a significant number of data and consumption of working time, there has been an increased need to use more complex data processing techniques from the mathematical point of view. Multivariate analysis was introduced a few decades ago in the treatment of chemical data and has been rapidly gaining popularity, giving rise to a new discipline called chemometrics. Multivariate methods consider the correlation between many variables analyzed simultaneously, allowing the extraction of a larger amount of information, often impossible to be obtained when analyzing variable by variable (Ferreira et al., 2002).

Some of these correlations are based on assessing external threats and opportunities and the company's internal predisposition to respond to these challenges and control the external environment, its strengths, its potentialities based on its resources, infrastructure, human capital and partnerships (Tigre, 2006). In this context, for companies to remain competitive, they seek to differentiate themselves through the search for innovation and the attempt to anticipate trends and signs of change, so that they can position themselves ahead of competitors in the market (Antunes et al., 2018).

Technological prospecting studies have a decisive place in reducing uncertainties and in strategic decision-making processes. Technological transformations, especially those that have happened in recent decades, point to the need to use information that can guide the future, information that prospective studies can provide. Coelho et al. (2005) describe that prospecting requires the identification of the most important opportunities and needs for research and development (R&D).

In this context, for Tigre and Kupfer (2004), technological prospecting is a disciplined way to map future scientific and technological developments that can significantly influence an industry, the economy or society as a whole, as well as showing what can succeed in terms of technological innovation.

Given this scenario of conciliation between technological modernization for laboratory analyses and the competitiveness of the market by companies that can expedite this process thus allowing a time gain in generating the final report containing the classification of the analyzed water sample, the present study aimed to present a prospective survey of studies on water classification, for irrigation purposes, in which chemometric methodologies were used. The prospecting considered the last decade, both in searches in scientific databases, for instance articles, and in public and private patent databases.

2. Methodology

This is a prospective and exploratory research, to know the scientific and technological development of the water quality classification methods that used chemometrics for data analysis and the determination of the class to which the analyzed sample belongs.

The search for scientific production on the theme was carried out in the portal of journals of the Coordination for the Improvement of Higher Education Personnel (CAPES) and in Scopus. Only research and review articles were analyzed in the advanced search of the databases, using filters to select relevant articles for the research and considering only peer-reviewed journals. For the search for patent applications, the national database of the National Institute of Industrial Property (INPI) and the international databases Espacenet and Orbit Intelligence were used.

In the investigations, a combination of keywords were used, applying Boolean operators, both in patent databases and in journal databases, always in the field of advanced search with the terms: “Water quality”, “Chemometrics”, “Water quality and classification”, “Classification and Chemometrics”, “Water Quality and Chemometrics” and “Classification of Water Quality and

Chemometrics" and the same terms in Portuguese for national databases, from January 2010 to January 2020. Subsequently, the obtained data were organized in visual representation, such as figures and tables, with the help of Microsoft Office Excel and Questel Orbit® software.

3. Results and Discussion

Based on the combination of keywords and the uses of Boolean operators, in the Periódicos Capes and Scopus databases, it was possible to create Table 1, which presents the quantities of articles that address the theme under study. Thus, of the databases explored, from the Periódicos Capes, Scopus had the largest number of journals for all keywords used, representing up to more than 50% of the results obtained.

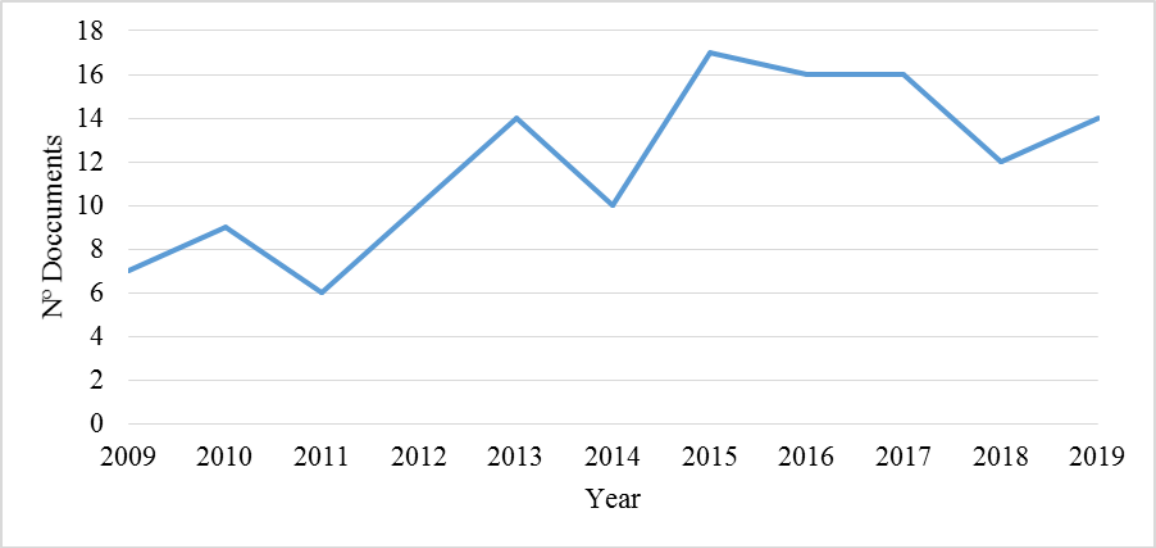
Table 1 - Quantity of Documents Found in Journal Databases According to the Keywords

Keywords	**Nº of articles**	
	Periódicos Capes (Portuguese)	**Scopus (English)**
Qualidade da água / Water quality	144,196	111,732
Quimiometria / Chemometrics	17,326	7,768
Qualidade da água AND classificação / Water quality AND classification	22,901	2,430
Classificação AND quimiometria / Classification AND chemometrics	5,824	1,596
Qualidade da água AND quimiometria / Water quality AND chemometrics	892	131
Classificação qualidade da água AND quimiometria / Classification water quality AND Chemometrics	13	12
Total	191,152	123,669

Source: Authors (2020).

When the search in the Scopus database was refined, by combining the words *water quality* AND *chemometrics*, 131 articles in this segment were obtained. Figure 1 presents the number of documents published per year, showing that publications became more representative from 2015, with the highest number of publications between 2015 and 2017, ranging from 16 to 17 documents per year.

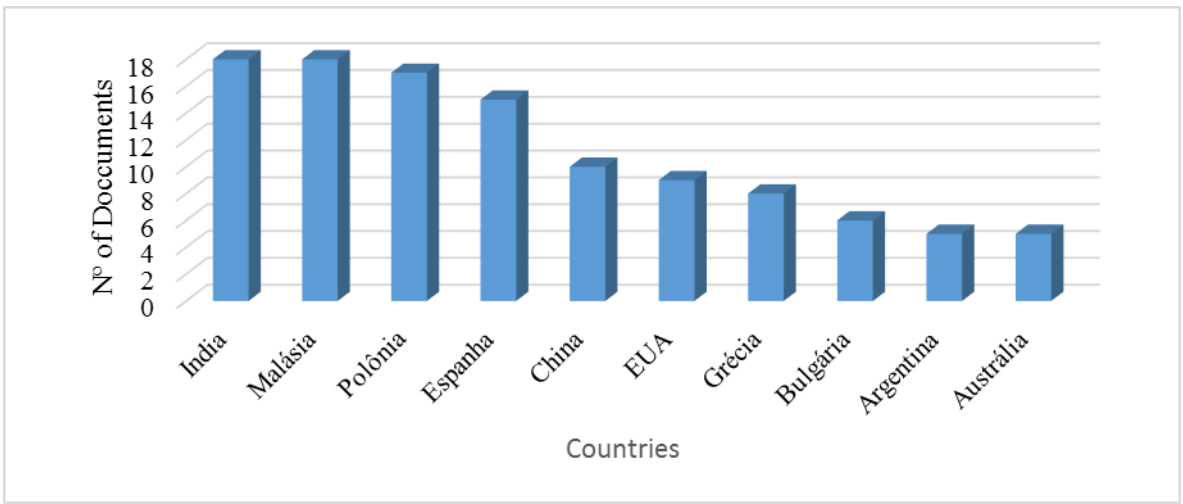
Figure 1 – Number of Articles Published in the Last Ten Years



Source: Authors (2020).

Figure 2, in turn, shows the countries that published significant numbers of articles between 2009 and 2019, with Poland standing out in first place with 17 articles and Malaysia in second place, with 16. China, which always stands out in terms of innovation, appears with 09 publications, in fifth place.

Figure 2 – Number of Articles published by Country of Origin



Source: Authors (2020)

With regard to the Research Institutions, Figure 3 presents the number of articles by the main publishing institutions, all of which are universities and/or research centers, with no company. The University of Malaysia is the affiliation with the highest number of articles, 7. Malaysia dominates

the publications, with 4 institutions with publications on *water quality* AND *chemometrics* between 2009 and 2019. These figures represent the country's interest in the development of equipment or their improvement in the assessment of water quality.

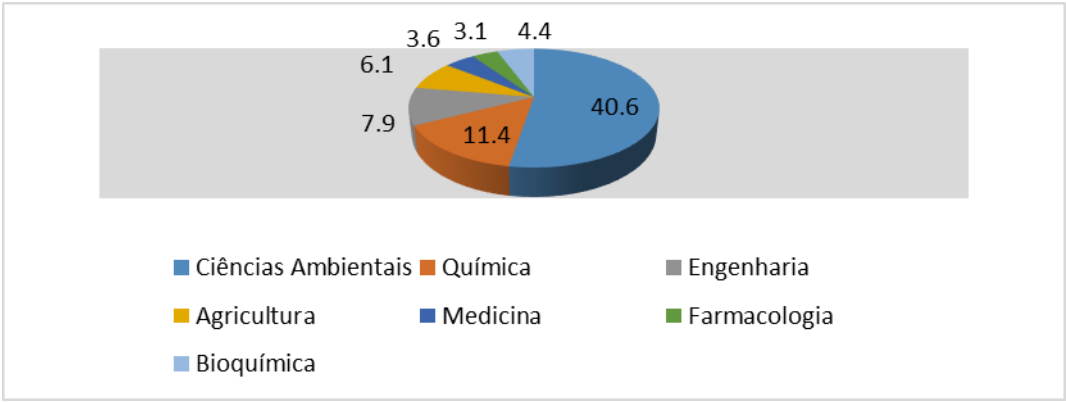
Figure 3 – Number of Articles Published by the most Productive Institutions

A - University of Putra Malaysia
B - University of Malaysia
C - National University of Malaysia
D - Chinese Academy of Sciences
E - CSIC- Spanish National Research Council
F - Sofia University – Bulgaria
G - Madras University –India

Source: Authors (2020).

Also regarding the data obtained by the search in Scopus with the keywords mentioned above, Figure 4 shows that most publications were carried out in the areas of environmental sciences, representing more than 40% of the studies on the subject, followed by chemistry (11.4%) and engineering (7.9%), which are the foundation for water quality studies.

Figure 4 – Number of Articles Published in the Last Ten Years per Area of Knowledge



Source: Authors (2020)

For the patent databases, the search was performed with the same keywords in Portuguese in INPI and in English in Espacenet. Brazil lacks patents in this area, as represented in Table 2, since INPI had a smaller number of documents filed, with zero results for most combinations of words in

the searches. For Orbit, the number of patents filed between 2010 and 2020 is quite significant, especially in comparison with the national database, as 31 documents were obtained in INPI and 95,171 documents were obtained Orbit for the general word *water quality*.

Table 2 – Quantity of Documents Found in Patent Databases According to Keywords

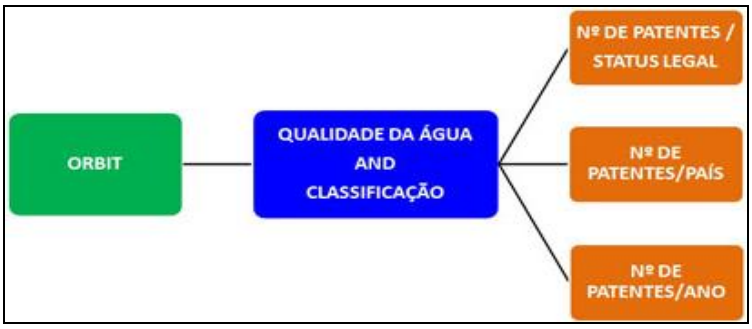
Keywords	**Nº of patents**		
	INPI (Portuguese)	**Espacenet (English)**	**ORBIT (English)**
Qualidade da água / Water quality	31	2,028,684	95,171
Quimiometria / Chemometrics	8	1,862	228
Qualidade da água AND classificação / Water quality AND classification	0	99,377	184
Classificação AND quimiometria / Classification AND chemometrics	0	548	25
Qualidade da água AND quimiometria / Water quality AND chemometrics	0	764	3
Classificação qualidade da água AND quimiometria / Classification water quality AND chemometrics	0	258	0
Total	39	2,032,116	95,611

Source: Authors (2020)

In the Espacenet database, results were obtained for all keyword combinations, with the highest number of results, 2,028,684 patents for the term *Water quality*. On the other hand, in the national database of INPI, the results were zero in four of the six related research categories (Qualidade da água AND classificação, Classificação and quimiometria, Qualidade da água and quimiometria, and Classificação qualidade da água and quimiometria), with very low values in the other search categories, when compared to the results obtained in the international database (Table 2).

Figure 5 illustrates the patent search method. It was decided to use Questel Orbit® software with the combination *Water quality* AND *chemometrics*. For a better result, the number patents filed per year, per country and the legal status of these patents in the last 10 years.

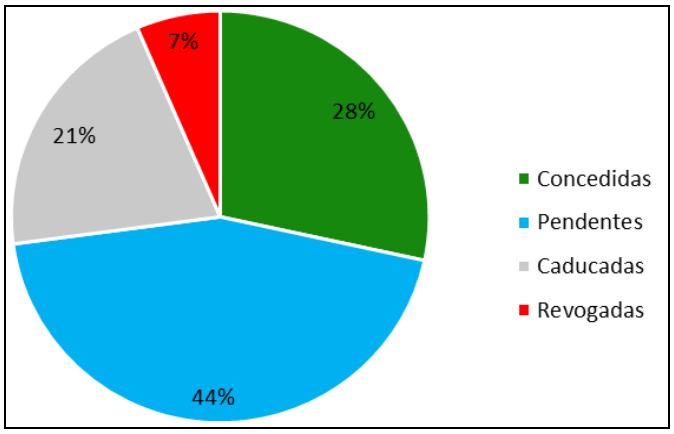
Figure 5 – Patent Search Method



Source: Authors (2020)

When analyzing the patent data, using Questel Orbit® software, it was possible to observe that, regarding the legal status of the patents filed, 28.4% of the patents were granted, 20.6% of the patents are expired, 44.5% are pending and 6.5% are revoked, as represented in Figure 6.

Figure 6 – Number of Patents Published from 2009 to 2019 by Country

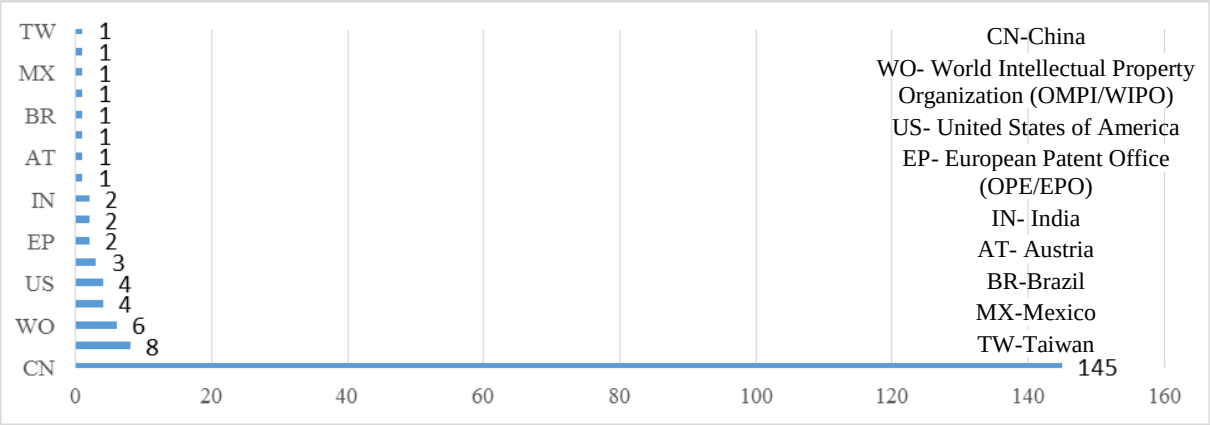


Source: Authors (2020).

According to Art. 30 of Law No. 13,243, of 01/11/2016, the patent application will be kept confidential for 18 (eighteen) months counting from the date of filing or the oldest priority, when there is, after which it will be published, except for the case described in Article 75. Thus, the high number of pending patents may reflect a considerable increase in the number of granted patents on the assessment of water quality in the coming years and even months of 2020.

With regard to countries, Figure 7 presents the number of patents published in the last ten years (2009-2019), and the highest one was obtained by China, which appears in first place with 145 patents, followed the United States in second with 04 patents. Brazil appears in position 7 of the list with only one patent.

Figure 7 – Number of Patents Published in the last Ten Years per Country

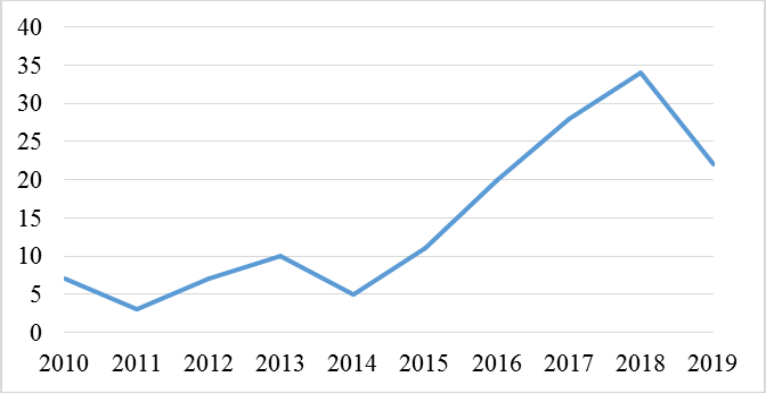


Source: Authors (2020)

In relation to the number of patents filed per year, for this same combination, the concentration of these documents in the last 05 years (2015-2019) is noticeable, as shown in Figure 6. Thus, it can be observed that there is no linearity, but that there are some technological peaks especially distributed in the last five years. The lack of linearity may be related to the periods of warming of the economy and the pace of the global welfare industry, since the theme involves technology, food and health of the population.

These technological peaks described in Figure 8 are not necessarily a consequence of investments in Research & Development (R&D), because it is worth mentioning that the models of innovation produced need to be approved by users, and non-acceptance may be responsible for the fluctuations of patent filings and consequent development of technologies, as shown for the year 2011, which had the lowest number of patents filed within this time interval analyzed (Menezes et al., 2018).

Figure 8 – Evolution of Patents in the last Ten Years



Source: Authors (2020)

4. Conclusions

From the scientific and technological prospecting carried out in this work, it was noticed that in the studied period there was an increase in the number of patents filed and articles produced, with regard to technologies involving chemometric analysis of water quality. On the other hand, Brazil has a deficit in this field, especially with regard to portable devices for the classification of a water sample according to CONAMA Resolution No. 357, of March 17, 2005. In the world, the country that stands out is China, which is mainly focused on the treatment and conservation of groundwater, presenting technologies to treat even hazardous solid waste, preventing it from polluting groundwater.

Therefore, this study showed a broad overview for investments, both public and private. Although there is a considerable number of scientific articles on the subject, the number of patents is very low.

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