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Teaching of Chemistry

Is the use of the Problem Based Learning Model by using Instagram effective to use? A Review

Mass spectrometry

variation in the chemical composition of essential oils from *Mangifera indica* L. leaves by comprehensive two-dimensional gas chromatography

Chemometrics

Multivariate statistical analysis of physicochemical parameters of groundwater quality using PCA and HCA techniques

Learning

Scientific recreations to favor the learning of the periodic table in high school students with incomplete schooling

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Editorial

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Editorial

In the fourth issue of Eclética Química, in 2023, readers will find important articles on chemistry education, groundwater quality and the rich chemical composition of volatile compounds contained in leaves of a medicinal plant. Opening this issue, a review presents how Instagram media can assist students to expand their critical thinking skills, solve problems, making the process fun, innovative, easy to understand, and not boring. The lack of motivation and comprehension of students make Chemistry be considered a difficult subject for them. According to this review, the application of the problem-based learning model in learning may help students to develop critical thinking skills and solve problems. Besides, the contents offer perspectives and innovations for teachers to deal with problems experienced by students. In the sequence, the analysis of different varieties of the same species demonstrates the different distribution of the volatile compounds present in leaves of *Mangifera indica* L. essential oils. The leaves of this plant have been used to treat diseases such as asthma, dysentery, cough, leucorrhea, jaundice, pain, and malaria. The use of comprehensive two-dimensional gas chromatography coupled to time-of-flight mass spectrometry allowed to identify 125 compounds in the variety 'espada' and 95 in the variety 'coração de boi', a considerable higher number than that until known. Following, it is presented a multivariate analysis of groundwater quality from different tubular wells by applying the techniques of principal component analysis (PCA) and hierarchical cluster analysis (HCA), which are powerful tools in the study of groundwater quality. Eleven parameters were analyzed of groundwater collected in two different seasons and both tools indicated a change in patterns between the analyzed periods. The correlation matrix corroborates the PCA data, and the HCA confirmed the correlations between the samples. Thus, it is feasible to assess the degree of similarity between the composition of the water from the different wells and between the parameters evaluated. Closes this issue a study that implements a didactic guide with scientific recreations to favor the learning of the periodic table, using an experimental, field, and explanatory research. For data processing, analysis, and interpretation the main theoretical and empirical methods were applied and allowed to conclude that the didactic guide with scientific recreations significantly improved students' learning of the periodic table.

The Editor and the Eclética Química Editorial team would like to render a special acknowledgement to the authors and reviewers for their effort, dedication to successful conclude not only this issue but all issues of this year with interesting articles leading with different subjects. Simultaneously, we kindly invite authors, readers, and reviewers to visit the Eclética Química page and contribute to the journal's next issues.

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Book
Hammond, C. *The Basics of Crystallography and Diffraction*, 4th ed.; International Union of Crystallography Texts on Crystallography, Vol. 21; Oxford University Press, 2015.

Book chapter
Hammond, C. Crystal Symmetry. In *The Basics of Crystallography and Diffraction*, 4th ed.; International Union of Crystallography Texts on Crystallography, Vol. 21; Oxford University Press, 2015; pp 99−134.

Book with editors
Mom the Chemistry Professor: Personal Accounts and Advice from Chemistry Professors Who Are Mothers, 2nd ed.; Woznack, K., Charlebois, A., Cole, R. S., Marzabadi, C. H., Webster, G., Eds.; Springer, 2018.

Website
ACS Publications Home Page. https://pubs.acs.org/ (accessed 2019-02-21).

Document from a website
American Chemical Society, Committee on Chemical Safety, Task Force for Safety Education Guidelines. *Guidelines for Chemical Laboratory Safety in Academic Institutions*. American Chemical Society, 2016. https://www.acs.org/content/dam/acsorg/about/governance/committees/chemicalsafety/publications/acs-safety-guidelines-academic.pdf (accessed 2019-02-21).

Conference proceedings
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PREPRINT
Fugivara, C. S.; Guilherme, L. H.; Benedetti, A. V. Microstructure of a passive film galvanostatically grown on stainless steel. ChemRxiv. [PREPRINT] September 20, 2021. https://doi.org/10.26434/chemrxiv.xxxxxx.v1 (accessed 2021-12-19).

Patent
Lois-Caballe, C.; Baltimore, D.; Qin, X.-F. Method for Expression of Small RNA Molecules within a Cell. US 7 732 193 B2, 2010.

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REVIEW ARTICLES

ORIGINAL ARTICLES

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Review article

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Is the use of the Problem-Based Learning Model through Instagram effective? A Review

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3. problem-based learning

ABSTRACT: Chemistry is still considered a difficult subject for students due to a lack of motivation and understanding. Implementing a problem-based learning (PBL) model with the media of Instagram can help students expand their critical thinking and problem-solving skills. To this end, 20 empirical research articles from inside and outside Indonesia were examined using the bibliometric analysis method to find research gaps and novelties as a basis for future research. The review shows various difficulties faced by students in studying chemistry. Instagram-based chemistry learning can help the learning process to be fun, innovative, easy to understand and not boring. Applying the PBL model to learning can help students develop critical thinking and problem-solving skills. The results of this analysis offer perspectives and innovations for teachers to deal with the problems faced by students, presenting innovations in learning, such as the use of Instagram and PBL models.

CONTENTS

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1. Introduction

Essentially, as time progresses, continuous development is inevitable. In light of this circumstance, it is necessary to improve the quality of human resources that can withstand the age of globalization. One of the efforts to improve the quality of human resources is education. In order to achieve the educational goals, it is necessary for the student to really pay attention to the study process in accordance with the applicable curriculum. In Indonesia, the 2013 curriculum is based on a scientific approach with four learning models, including discovery, inquiry, problem-based and project-based learning. What teachers need to do when implementing the 2013 curriculum is to help students develop habits so that they can always increase their awareness of learning, because the 2013 curriculum is applied based on existing problems. For this reason, students are expected to actively participate in the learning process (Sariono, 2013).

Problem solving is part of the reasoning process. This process is generally considered to be the most complex of all the characteristics of intelligence and can be interpreted as a higher-order cognitive process that requires more coordination and control of routines or other basic skills. Problem-solving skills include critical, logical and systematic thinking. An integrated teaching process can help students develop the ability to express and execute them in real life and relate what they have learned to life experiences. Thus, education should focus on improving skills and unleashing students' creativity to solve problems. The problem presented is usually taken from the real world, as a context for students to practice critical thinking and problem solving (Amir, 2009).

Memnun *et al.* (2012) found that the main goal and priority in education today is to train students to be more flexible in solving problems and to deal with all the problems they face. This shows that problem-solving skills play a very important role in the world of education. Hamiyah and Jauhar (2014) suggested that the indicators of problem-solving skills are divided into four parts: understanding the problem, planning the solution, dealing with the problem according to the plan created and re-examining all the steps.

Chemistry presents itself as a complex scientific discipline encompassing the examination of matter's structure, composition, properties, and the alterations it undergoes, often involving energy transformations. The difficulties experienced by students in studying chemistry can be attributed to the inherent complexities of this field. Prilianti (2012) suggested that chemistry has characteristics that are mostly abstract, sequential, and fast-developing concepts. He also proposed that difficulties in understanding the subject are rooted in problems understanding chemical concepts.

One of the chemistry subjects studied in Indonesian high schools is reaction rate. Sudarsana (2010) stated that the reaction rate subject taught there is still taught through lectures or memorization of most reaction rate concepts. This encourages teachers to apply the problem-based learning (PBL) model to the concept of reaction rate, because the material factors that affect reaction rate are closely related to the real world. In addition, the PBL model can also involve students in being active in the classroom, collaborating and finding solutions to the problems being studied. It is expected that the active participation of all students in their learning and the enhancement of their critical thinking skills will improve their learning outcomes, especially cognitive learning outcomes.

While learning and teaching chemistry, the usefulness of a teaching model determines student interest and success. The use of an inappropriate teaching model is a factor that makes learning chemistry difficult for students. They feel that what they learn is not related to their everyday lives. Chemistry is abstract and requires student activity to solve various chemistry-related problems.

A PBL strategy encompasses a series of learning activities. In short, it requires students to learn through PBL, rather than simply listening, taking notes, and memorizing information. With such strategies, they are proactive in thinking, communicating, researching, and reprocessing, entering data and finally completing it. In addition, problem-solving is done by applying scientific approaches. Thinking scientifically is a deductive and inductive thought process. The fact that the thinking process is carried out systematically means that scientific thinking is performed at a specific stage, and empirically means that the problem-solving process is performed with clear data.

Based on the characteristics of the reaction rate subject, Instagram-assisted PBL can be carried out. The number of Instagram users in Indonesia in 2020 reached 99.9 million people (Siahaan *et al.*, 2022). The most important reason for using Instagram as a learning medium is that students are familiar with its use. Since almost all students already have laptops and gadgets and still use Instagram, more educators do not have to pay much to apply it. It is also easy to apply, as it is an app that can be used anywhere. It is also easy to use, as it does not require any special training.

Furthermore, there are several reasons to consider Instagram as a learning medium: 1) Instagram can be used at all levels of education; 2) Instagram gives

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students the authority to create digital content on their own and publish it online, which can stimulate student and educator activity in teaching; and 3) Instagram allows collaboration between students and educators on a specific project or task to achieve learning objectives.

Structured learning based on PBL syntax, whose content consists of text, images, or videos or all three, is accompanied by instructions that students can use independently in their learning, without being limited by space and time. Indah (2021) proposed that, in relation to students' needs and characteristics, 94.4% of them use the Internet frequently to do tasks and understand content. Based on the results obtained in this study, the same percentage of students often use and like the social media Instagram.

Sujiono and Widiyatmoko (2014) suggested that PBL is very effective in expanding students' ability to think critically. The subject of reaction rate is closely related to counting. Jayadiningrat and Ati (2018) used a PBL model in chemistry learning and found that the application of this PBL can improve problem-solving skills in chemistry subjects, recognizing and formulating the problem, exploring alternative solutions, choosing the best solution and solving problems smoothly.

Oktaviani *et al.* (2017) found that using PBL as a learning model on the concept of reaction rate has a very good effect on the creativity aspects of students. Through PBL activities, students who acquire knowledge from discoveries made in the problem observation phase in the form of practical images and videos gradually begin to construct all the information found and obtained into their thinking patterns.

Social media has not been widely used for learning purposes, but this is an effort to make learning activities more fun and learning objectives achievable. The use of Instagram can have a positive impact on improving students' learning skills and understanding. Uploads made on Instagram can be visualized and displayed in feeds that can be viewed by Instagram followers and researchers in general. Instagram users can interact and chat with each other by commenting on or liking the uploaded photos and videos that have been published. Meanwhile, to interact privately, Instagram also offers a chat feature that is commonly referred to as a direct message or DM. Instagram can be used on various devices, such as smartphones, laptops and so on (Ambarsari, 2021).

The features available on Instagram really support the learning process: such as the TV function, which can deliver materials from 1 to 60 minutes; the Feed Post function, which can publish an overview of the material to be delivered; there is a background sound option that can be used to increase students' enthusiasm; the live feature, which is used by users who are doing activities and want to interact with their followers, as if they were talking directly to them and the audience that can be answered via chat (Al Mardhiah *et al.*, 2021).

Instagram's Stories feature consists of a 15-second photo or video upload that will automatically disappear within 24 hours, unless the upload is inserted into the Highlights on the Instagram account profile. In Instagram's Highlights feature, it is possible to create groups of Stories according to their categories. This makes it easier for students to review learning materials. Instagram also offers a variety of interesting music that can be used as a background. The use of such music can also increase students' interest in learning (Al Mardhiah *et al.*, 2021).

This is in line with the research on Instagram as a learning medium, which shows that the use of Instagram-based learning can increase student motivation, as the features of Instagram are diverse and interesting, which makes it easier for students to understand (Fidian, 2017). Irwandani and Juariyah (2016) suggested that those who use Instagram in their research show that developing products with the help of this social network is feasible, effective and can be used as an alternative for learning, as it can be accessed anytime and anywhere. Therefore, this study aims to provide a literature review to analyze the use of Instagram for learning purposes, including PBL models. The following is the main research question that this study seeks to answer: Is the use of the PBL model using Instagram effective for use in the chemistry learning process?

2. Experimental

The method used to complete this article using the bibliometric literature or article review method. The use of bibliometric analysis techniques can provide an accurate and objective way of measuring an article's contribution to the advancement of knowledge and is a commonly used tool for analyzing trends and performance on a particular subject (Yang *et al.*, 2013). Bibliometric analysis is a common method for investigating and analyzing large amounts of scientific data. Bibliometric analysis is used in the hope of finding research gaps and novelties as the basis for further research.

The bibliometric method of literature review was used to prepare this article. Bibliometric analysis techniques can provide an accurate and objective way of measuring an article's contribution to the advancement of knowledge and are commonly used tools for analyzing

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trends and the performance of a given subject. Bibliometric analysis is a common method for investigating and analyzing large amounts of scientific data and is used in the hope of finding research gaps and novelties that serve as a basis for new research (Yang *et al.*, 2013).

The researchers investigated journal articles on the effectiveness of learning through Instagram on the grounds of a PBL approach in the context of reaction rate. This research used 20 national and international articles through a search on the Google Scholar platform. The articles used have undergone similar research and were analyzed and summarized. The results of the research are summarized in this article for discussion.

According to Tranfield *et al.* (2003), the method used in this study consisted of five steps, namely.

2.1 Determine the keyword

In this study, the keywords used to search for related literature in Google Scholar using Publish or Perish 7 software were "the application of Instagram media in learning," "the effectiveness of Instagram media in learning," and "Problem-Based Learning (PBL) on reaction rate material."

2.2 Literature data selection

This was done by reading the title of each article on the research topic when selecting the bibliographic data. As a result, there were references that did not correspond to the research topic, so the inappropriate articles were excluded and the appropriate results were returned: "the use of Instagram media in learning" as many as 60 articles, "the effectiveness of Instagram media in learning" as many as 14 articles, and "Problem-Based Learning (PBL) based on the reaction rate material" as many as 40 articles.

2.3 Literature data extraction and analysis

Bibliometric analysis was performed using VOSviewer software. Obtain around 20 journal articles related to the theme, which are then analyzed for the content and intent of these articles.

3. Results and discussion

The results of the research data contained in this literature review are an analysis and summary of the articles on PBL in the application of Instagram in learning, the effectiveness of this social media (Tables 1, 2 and 3).

Table 1. Research results related to the application or implementation of Instagram media in learning.

Researcher	Research Title	Research result
Muhtar *et al.* (2017)	The two blended learning model designs (Moodle and Instagram): A comparative study in university level	This can improve students' skills, self-control, and motivation
Salehudin *et al.* (2017)	Using Instagram to support creative learning and project-based learning	Can be freely used to improve students' creative and high order thinking skills
Ambarsari (2021)	The use of Instagram as a media for learning Indonesian language and literature in Era 4.0	Learning with Instagram becomes easier for teachers and students, so students can interact freely remotely, but the materials they share with them can be properly delivered
Qisthi and Arifani (2020)	The application of project-based learning via Instagram to improve EFL students' speaking skill	Can improve students' declaring, speaking, or pronouncing skills
Astuti (2021)	Distance learning media using Instagram as a learning tool to express students' opinions	Instagram is quite effective to be used as an alternative media for learning at all levels
Dewi *et al.* (2021)	Implementation of the utilization of Google Classroom, Google Meet, and Instagram in the online learning process towards the 21st century	It can make online learning activities easier for teachers and students. Learning that integrates the three media can provide character education for discipline, activeness, achievement of creativity, information literacy, collaboration, and responsibility
Sari (2021)	Utilization of learning media using the "Instagram Reels" feature in Indonesian language and literature learning during the COVID-19 pandemic	It helped educators or teachers to conduct online (online) learning. Because the features offered by Instagram Reel meet their learning needs

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Table 2. Research on the effectiveness of Instagram media in learning.

Researcher	Research title	Research result
Irwandani *et al.* (2020)	Effectiveness of physics learning media course assisted by Instagram on student's creative thinking skill	Learning with social media, especially Instagram, is said to be effective for students' creative thinking skills. This result is also consistent with responses from students who were rated "good" for studying Physical Learning Media (PLM) courses using social media Instagram
Pratiwi (2019)	The effectiveness of media Instagram toward the students' speaking skills of 10th Grade State Senior High School 4 Malang	State Senior High School 4 Malang's X-Class students have a significant impact on Instagram media's speaking skills, which is indicated by pre- and post-test scores
Lubis *et al.* (2020)	The effectiveness of using Instagram as teaching tools in learning process of 3rd semester of English Department students	Instagram is one of the most effective social media that can be used as a platform for educational and learning processes. Instagram was also effectively used as a means of student interaction, especially in discussions related to task activities and explanations
Sinatrya and Aji (2020)	The effectiveness of the online flipped classroom learning model using Instagram in Class X Vocational High School	Instagram in the learning process can be effective using the flipped classroom method. Using Instagram as a learning model is a new experience for students, and it is easy for them to access and use

Table 3. Research results related to PBL on reaction rate material.

Researcher	Research title	Research result
Oktaviani *et al.* (2017)	Implementation of the problem-based learning model on the creativity of students in the material of reaction rates at State Senior High School 4 Banda Aceh	The application of the PBL learning model can improve and develop the creativity of students
Zahrah *et al.* (2017)	Application of practicum with problem-based learning (PBL) Model on reaction rate material at State Senior High School 1 Lembah Selawah	PBL model with practicum method can improve students' high order thinking skills on the concept of reaction rate chapter and improve students' scientific attitude
Utami *et al.* (2018)	The influence of problem-based learning (PBL) learning model on cognitive learning outcomes of Class XI Students of State Vocational High school 02 Manokwari (study on the main material of the reaction rate concept)	The percentage of the effect by implementing PBL has a 30% effect on student cognitive learning outcomes
Dakabesi and Luoise (2019)	Effects of problem-based learning models on critical thinking skills in the context of reaction rate	This can improve students' critical thinking skills and academic ability
Mayasari *et al.* (2019)	Comparison of problem-based learning and guided inquiry learning models on critical thinking ability in reaction rate materials	Learning with these PBL models has shown that students have higher critical thinking skills than with guided query learning models
Nangku and Rohaeti (2019)	The effect of problem-based learning model toward students conceptual understanding and verbal communication skills in reaction rate learning	PBL models have a positive impact on student learning outcomes in terms of conceptual comprehension and language communication skills
Redhana *et al.* (2019)	Development of scientific learning devices with problem-based learning models through inductive reasoning on the topic of reaction rate	The PBL model, in addition to improving problem-solving skills, helps students in constructing various existing problems into new knowledge, that is easily understood by students
Suarningtyas and Hidayah (2022)	Development of student e-worksheet based on problem-based learning to practice metacognitive abilities of high school student on reaction rate material	PBL students can train metacognitive abilities on the reaction rate material

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3.1 Application and effectiveness of using Instagram media in learning

Atmoko (2012) suggests that Instagram is a popular social media application for the public, including students. Instagram can inspire and develop creativity for its users because it has photo and video editing features that make it better and more attractive. The media used by the teacher is limited to textbooks, which is less interesting for students so that their motivation in reading the subject matter is very low. Therefore, we need media that can increase interest in learning so that students can improve their problem-solving skills.

The popularity of Instagram makes it effective to be used as a studying platform. That advantage of Instagram as a learning-based media, compared to other ones, is that it is more interesting, it is accompanied by illustrations, pictures, it is accessible anytime and anywhere, easy to use, and has no limit on the number of users. Nastiti (2019) proposed that Instagram can help teachers delivering subject matter, improving learning outcomes, helping students understand the material, and attracting students' attention—so that this platform is suitable for use as a learning medium.

Based on the findings in Tables 1 and 2, the surveys conducted received positive feedback from students. But despite that, Instagram has also its drawbacks. The disadvantages are: (i) too free to access, so students would need parental supervision; (ii) need for a stable Internet network, because if there is an Internet failure, the learning process will slow down a bit.

Based on the results contained in Table 1, the findings on implementation of this application were called effective. Muhtar *et al.* (2017) have shown its support in teaching and learning activities. In this case, students could improve their language proficiency, skills, self-discipline, and motivation. Their study aimed to determine the effectiveness of blended learning using two different media (i.e., Instagram and Moodle) for two different subjects (Mathematics and English Expression). Salehudin *et al.* (2017) discovered, by implementing Instagram media, that students improved creative and critical thinking skills. Their study aimed to examine this effect through the interaction of study models aided by Instagram and user experience related to conceptual understanding.

Ambarsari (2021) proposed that Instagram can be used as a learning medium, especially in learning Indonesian language and literature. Instagram makes it easier for teachers and students to interact remotely, with study material being properly notified and communicated. This study aimed to establish the viability of the Instagram app as a medium for language and literature learning. For Qisthi and Arifani (2020), Instagram can be a fun and effective tool for learning language skills. This study aimed to examine the impact of using Instagram on improving students' speaking skills.

Astuti (2021) proposed that the use of Instagram in learning is quite effective as an alternative learning media at all levels. This study aimed to determine freedom of expression in social media and examine the use of Instagram for learning by students in class XI Vocational School in Padang. Dewi *et al.* (2021) found that Instagram can be convenient for teachers and students in remote learning activities. Learning that integrates Google Classroom, Google Meet and Instagram can provide character building for discipline, activity, the achievement of creativity, information literacy, collaboration, and responsibility. This study aimed to propose innovations during learning methods to achieve students' cognitive, psychomotor and character traits based on information and communications technology.

Sari (2021) proposed that the Instagram Reels feature in Indonesian language and literature learning can help educators develop online learning resources that are in line with Indonesian language and literature learning needs. The advantages of the Instagram Reels feature are also considered to be more dominant than its weaknesses. This study aimed to find out whether the Instagram Reels feature in Indonesian language and literature learning can help online learning.

Irwandani *et al.* (2020) found that learning physics lessons supported by Instagram were effective for students' creative thinking skills. This result is also consistent with the response of the student who rated her Physical Learning Media (PLM) course as "good" through Instagram. The aim of this study was to determine the effectiveness of Instagram-enabled PLM learning and to determine the impact on students' creative thinking skills.

Pratiwi (2019) suggested that Instagram had a significant impact on the speaking skills of Class X students at Malang State High School 4, as evidenced by the pre- and post-test results. The aim of this study was to determine the effectiveness of using Instagram for these students' speaking skills. Lubis *et al.* (2020) found that Instagram is also used effectively as a means of student interaction, especially in activity-related discussions and task explanations. In addition, almost all students use this app, so they find it easier to use. The aim of this study was to examine the effectiveness of implementing Instagram in distance teaching and learning. Sinatrya and Aji (2020) proposed using this

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flipped classroom learning model to determine the effect of implementing Instagram on the learning process. This was evidenced by the significant increase before and after the test. The authors considered that using Instagram as a learning tool is a new experience that is easy for students to access and use.

The aspects that need to be considered in the effectiveness of Instagram learning are: (i) Instagram should contain useful content with high creativity; (ii) the content contained makes it easier for students to capture abstract ideas or formulations; (iii) it develops students' interest in reading and other fields of study; (iv) it helps students understand a subject considered difficult by creating content with easy-to-understand vocabulary. There are several reasons to use Instagram for research, education and study, including: (i) easy access (it can be accessed anywhere and at any time); (ii) most people, especially students and university students, have Instagram; (iii) the resources available are diverse; (iv) the duration of some resources is long enough, so it can be used to transmit material; (v) it can facilitate the interaction of educators and students.

3.2 PBL on reaction rate material

PBL is a learning approach in which students are presented with practical problems. The PBL model has been shown to explain the improvement of students' problem-solving and critical thinking skills. Students learning this approach observe the expertise present or try to discover the expertise they want in order to solve the problems they discover. Mahyana (2018) proposed that PBL be used as a learning model that can activate learning activities even when students are faced with problems that can stimulate critical thinking skills. Learning can be more meaningful and enhanced when students are presented with situations in which the concept applies.

In PBL, higher-order thinking skills are more required, because students are faced with a problem that requires them to solve it based on their ability to organize all their knowledge and experience, as well as the external conditions that are available or accessible. Rusman *et al.* (2010) proposed the following characteristics of the PBL model: (i) The problem is the starting point for learning; (ii) The problem posed exists in the real world and is unstructured; (iii) The problem increasingly requires multiple perspectives; (iv) The problems challenge the students' knowledge, attitudes and skills, which requires the identification of new areas of learning, mainly self-directed learning (v) Use of multiple sources of knowledge and information; (vi) Learning is collaborative, communicative and collaborative; (vii) The development of research and problem-solving skills is identical to the acquisition of knowledge to find solutions to problems; (viii) Integration of the learning process; (ix) PBL includes evaluation and review of the student and user experience of the learning process.

Based on the survey results shown in Table 1, the data from the survey conducted shows positive feedback from the students. The implementation of PBL models in the learning of kinetic chemistry of materials is very effective in applications. Oktaviani *et al.* (2017) found positive results with the implementation of the PBL model in the subject of reaction rate, in which the students' creativity obtained an average value of 92, which is categorized as very good, which shows that the students' creativity developed well after the implementation of PBL models in a chemical kinetics class. The aim of this study was to explain the students' creativity after implementing the PBL model in the reaction rate subject material.

Utami *et al.* (2018) showed that 30% of the results came from implementing PBL models in experimental classes. The objectives of this study were to find differences in cognitive learning outcomes between students taught through PBL and conventional learning and to find out how much the PBL model affects the cognitive learning outcomes of Class XI grader State Vocational High School 02 Manokwari.

Zahrah *et al.* (2017) found that PBL, as a model that uses practical techniques, can enhance students' critical thinking about this reaction rate concept and improve their scientific attitudes. This study aimed to determine the effectiveness of PBL models with practical techniques in improving students' critical thinking.

Dakabesi and Luoise (2019) suggested that students who learned in experiential classes were better at critical thinking than those who learned using traditional models. This study aimed to measure the effectiveness of improving students' critical thinking skills using PBL models. Mayasari *et al.* (2019) suggested that learning using the PBL model resulted in students' higher critical thinking skills than using the guided exploratory learning model. The aim of this study was to investigate learning models between PBL and guided questions that would best serve as response rate features in students' critical thinking skills.

Nangku and Rohaeti (2019) suggested that the implementation of a PBL model positively affects students' learning outcomes in terms of conceptual understanding and verbal communication skills. The aim of the article was to determine the impact of applying a project-based learning model on students' conceptual understanding and language skills when learning about

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reaction rate. Redhana *et al.* (2019) found that the PBL model, in addition to improving problem-solving skills, also helped students transform various existing problems into new knowledge that was easily understood by them. The aim of this research was to advance and represent the characteristics of learning devices that communicate with PBL models through prolegomenon reasoning on the topic of reaction rate.

Suarningtyas and Hidayah (2022) suggested that the Student E-Worksheet Based on PBL could train students' metacognitive skills in reaction rate material. Arends (2008) proposed three learning outcomes achieved by students taught with PBL: (i) research and problem-solving skills; (ii) learning adult role behavior; and (iii) suggested independent learning skills. Through problem-solving, students are empowered to use their logical reasoning, problem-solving and higher intellectual skills. Ultimately, PBL educates students to become independent learners. Improving their problem-solving skills can be very useful in life, as they develop the ability to deal with any problem in the environment.

There are certainly advantages and disadvantages to implementing PBL in the learning process. The benefits of PBL include: (i) problem solving can be a very effective and excellent technique for improving students' understanding; (ii) it can also be satisfactory for improving students' skills and expanding their knowledge; (iii) PBL can bring joy to students when solving problems; (iv) it can give students the opportunity to apply their knowledge in the real world. On the other hand, the weak points of applying problem-solving learning are: (i) that even when students are not interested or believe that the problem, they are studying is difficult to solve; (ii) they do not understand why they are trying to solve the problem; (iii) there is reluctance to solve problems when they are not at hand; and (iv) when they study, they do not learn what they want to learn.

4. Conclusions

Based on the results of the observations and discussions presented, it can be concluded that applying the PBL model to Instagram-based chemistry learning is effective. Observations from various studies on the use of PBL models show that it can improve critical thinking skills, solve provided problems and help students understand material more easily, because students do not just record, visualize, and memorize, but are required to actively form new knowledge through the problem-solving process. In addition, the use of Instagram in learning can also have a positive influence, increasing creativity and helping students to communicate the subject matter in a concise and easy-to-understand way using the resources provided. However, the application of a PBL model using Instagram also has several weaknesses, such as the need for a stable internet connection and, if students find it difficult to understand the problems presented, they tend to be lazy about finding solutions to these problems.

Authors' contribution

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References

Al Mardhiah, N.; Maulina, S.; Prasetyo, S. K. Pemanfaatan Media Sosial Instagram dalam Pembelajaran Bahasa Indonesia di Tingkat Perguruan Tinggi: Sebuah Gagasan Konseptual. *Prosiding Seminar Nasional Sastra, Pedagogik, dan Bahasa*. **2021**, *3* (1), 236–246.

Ambarsari, Z. Penggunaan Instagram sebagai media pembelajaran bahasa dan sastra Indonesia pada era 4.0. In: Prosiding Seminar Nasional Pembelajaran Bahasa

Eclética Química, vol. 48, n. 4, 2023, 17-26
ISSN: 1678-4618
DOI: 10.26850/1678-4618eqj.v48.4.2023.p17-26

dan Sastra Indonesia (SemNas PBSI)-3. FBS Unimed Press, 2021. p. 81-86. http://digilib.unimed.ac.id/id/eprint/41225 (accessed 2022-11-10).

Amir, T. Inovasi Pendidikan Melalui Problem-Based Learning. Prenada Media Group, 2009.

Arends, R. I. *Belajar Untuk Mengajar* (Terjemahan Helly Prajitno Soetjipto & Sri Mulyantini Soetjipto); MeGraw Hils, 2008.

Astuti, I. I. Media Pembelajaran Jarak Jauh Menggunakan Instagram sebagai Sarana Belajar Mengungkapkan Pendapat Peserta Didik. *Jurnal Pancasila dan Kewarganegaraan.* **2021**, *6* (2), 12–22. https://doi.org/10.24269/jpk.v6.n2.2021.pp12-22

Atmoko, B. *Instagram Handbook Tips Fotografi Ponsel* Media Kita, 2012.

Dakabesi, D.; Luoise, I. S. Y. The Effect of Problem-Based Learning Model on Critical Thinking Skills in The Context of Chemical Reaction Rate. *J. Educ. Learn*. **2019**, *13* (3), 395–401. https://doi.org/10.11591/edulearn.v13i3.13887

Dewi, K.; Pratisia, T.; Putra, A. K. Implementasi Pemanfaatan Google Classroom, Google Meet, dan Instagram dalam Proses Pembelajaran Online Menuju Abad 21. *Jurnal Integrasi Dan Harmoni Inovatif Ilmu-Ilmu Sosial.* **2021**, *1* (5), 533–541. https://doi.org/10.17977/um063v1i5p533-541

Fidian, A. Pengaruh Penggunaan Instagram Sebagai Media Pembelajaran Terhadap Peningkatan Motivasi Menulis Mahasiswa. *Jurnal Perspektif Pendidikan.* **2017**, *11* (2), 8–14.

Hamiyah, N.; Jauhar, M., *Strategi Belajar-Mengajar di Kelas*. Prestasi Pustaka, 2014.

Indah. Pengembangan-Komik Kimia Berbasis Etnosains Berbantuan Instagram Pada Materi Koloid. Ph.D. Thesis, University of Jambi, Indonesia, 2021. https://repository.unja.ac.id/id/eprint/21269 (accessed 2022-11-10).

Irwandani, M.; Juariyah, S. Pengembangan Media Pembelajaran Berupa Komik Fisika Berbantuan Sosial Media Instagram sebagai Alternatif Pembelajaran. *Jurnal Ilmiah Pendidikan Fisika Al-Biruni*. **2016**, *5* (1), 33–42. https://doi.org/10.24042/jpifalbiruni.v5i1.103

Irwandani, M.; Pricilia, A.; Sari, P. M.; Anugrah, A. Effectiveness of Physics Learning Media Course assisted by Instagram on Student's Creative Thinking Skill. *J. Phys.: Conf. Ser.* **2020**, *1467* (1), 012006. https://doi.org/10.1088/1742-6596/1467/1/012006

Jayadiningrat, M. G.; Ati, E. K. Peningkatan Keterampilan Memecahkan Masalah melalui Model Pembelajaran Problem-Based Learning (PBL) pada Mata Pelajaran Kimia. *Jurnal Pendidikan Kimia Indonesia.* **2018**, *2* (1), 1–7. https://doi.org/10.23887/jpk.v2i1.14133

Lubis, S. I. S.; Rayani, F.; Salmiah, M. The Effectiveness of Using Instagram as Teaching Tools in Learning Process of 3rd Semester of English Department Students. *Jurnal Bahasa Lingua Scientia*. **2020**, *12* (2), 217–228. https://doi.org/10.21274/ls.2020.12.2.217-228

Mahyana. Penerapan Model Problem-Based Learning untuk Meningkatkan Keterampilan Berpikir Kritis Siswa pada Kelas IV MIN 25 Aceh Besar. Ph.D. Thesis, State Islamic University Ar-Raniry, Indonesia, 2018.

Mayasari, A.; Fazli, R.; Rahmayani, I. The comparison of problem-based learning and guided inquiry learning model to the critical thinking ability in rate reaction. *J. Edu. Sci*. **2019**, *5* (1), 57–69. https://doi.org/10.3314/jes.v5i1.360

Memnun, D. S.; Akkaya, R.; Hacıomeroglu, G. The effect of prospective teachers problem solving beliefs on self-efficacy beliefs about mathematical literacy. *Journal of College Teaching and Learning Fourth Quarter.* **2012**, *9* (4), 289–298. https://doi.org/10.19030/tlc.v9i4.7299

Muhtar, S. N.; Kariadinata, R.; Rahayu, Y. N.; Laelatulatifah, A. The two blended learning model designs (Moodle and Instagram): A comparative study in university level. *2nd International Conference on Sociology Education.* **2017**, *2*, 303–307. https://doi.org/10.5220/0007108609430947

Nangku, M. S; Rohaeti, E. The Effect of Problem-Based Learning Model toward Students' Conceptual Understanding and Verbal Communication Skills in Reaction Rate Learning. *J. Phys.: Conf. Ser.* **2019**, *1397* 012037. https://doi.org/10.1088/1742-6596/1397/1/012037

Nastiti, R. Pengembangan Media Pembelajaran Komik Fisika SMA Berbasis Instagram dengan Aplikasi *Comic*

Eclética Química, vol. 48, n. 4, 2023, 17-26
ISSN: 1678-4618
DOI: 10.26850/1678-4618eqj.v48.4.2023.p17-26

Life pada Pokok Bahasan Gerak Lurus. Ph.D. Thesis, SKRIPSI Jurusan Fisika Fakultas, Indonesia, 2019.

Oktaviani, C.; Nurmallah, C.; Mahidin, D. Implementasi Model *Problem-Based Learning* Terhadap Kreativitas Peserta Didik pada Materi Laju Reaksi di SMAN 4 Banda Aceh. *Jurnal Pendidikan Sains Indonesia*. **2017**, *5* (1), 12–19.

Pratiwi, M. F. The effectiveness of media Instagram toward the students' speaking skills of Tenth Grade In SMAN 4 Malang. *J. Chem. Inf. Model*. **2013**, *53* (9), 1689–1699.

Prilianti, R. Pengembangan Perangkat Pembelajaran Pendalaman Materi Kimia Redoks Berbasis Empat Pilar Pendidikan melalui Lesson Study. Artikel Tesis, Universitas Negeri Semarang, 2012.

Qisthi, N.; Arifani, Y. The Application of Project based Learning via Instagram to Improve EFL Students' Speaking Skill. *Proceedings of the Borneo International Conference on Education and Social Sciences (BICESS 2018)*. 2020, 201-209. https://doi.org/10.5220/0009018802010209

Redhana, I. W.; Sudria, I. B. N.; Suardana, I. N.; Suja, I. W.; Haryani, S. Students satisfaction index on chemistry learning process. *Indones. J. Sci. Educ.* **2019**, *8* (1), 101–109. https://doi.org/10.15294/jpii.v8i1.15331

Rusman, E.; van Bruggen, J.; Sloep, P.; Koper, R. Fostering Trust in Virtual Project Teams: Towards a Design Framework Grounded in a Trust Worthiness ANtecedents (TWAN) Schema. *Int. J. Hum. Comput. Stud.* **2010**, *68* (11), 834–850. https://doi.org/10.1016/j.ijhcs.2010.07.003

Salehudin, M.; Sarimin, D. S.; Rondonuwu, R. H. S.; Yunus, M.; Safiah, I. Using Instagram to support creative learning and project based learning. *International Journal of Advanced Science and Technology*. **2020**, *29* (5), 4866–4876.

Sari, A. D. Pemanfaatan Media Pembelajaran dengan Menggunakan Fitur "Reels Instagram" pada Pembelajaran Bahasa dan Sastra Indonesia. *Prosiding Seminar Nasional PBSI-IV Tahun 2021 Tema: Pembelajaran Bahasa dan Sastra Indonesia Berbasis Digital Guna Mendukung Implementasi Merdeka Belajar. pp.* 2021, 33–38.

Sariono. Kurikulum 2013: Kurikulum Generasi Emas. *Jurnal Pendidikan*, **2013**, *3* (2).

Siahaan, C.; Salomo, S.; Adrian, D. Media Sosial Instagram sebagai Sarana Berkomunikasi di Lingkungan Masyarakat. Jurnal Ilmiah Ilmu Pendidikan. **2022**, *5* (8), 2843–2848. https://doi.org/10.54371/jiip.v5i8.774

Sinatrya, P.; Aji, S. U. Efektivias Model Pembelajaran Flipped Classroom Daring Menggunakan Media Sosial Instagram di Kelas X SMK. *Primatika. J. Pend. Mat.* **2020**, *9* (2), 81–90. https://doi.org/10.30872/primatika.v9i2.368

Suarningtyas, S.; Hidayah, R. Development of Student E-Worksheet Based on PBL (Problem-Based Learning) to Practice Metacognitive Abilities of High School Student on Reaction Rate Material. *Int. J. Curr. Sci. Res. Rev*. **2022**, *5* (5), 1680–1687. https://doi.org/10.47191/ijcsrr/V5-i5-35

Sudarsana, M. Pembuatan Program Pembelajaran Interaktif Laju Reaksi Berbantuan Komputer untuk Pembelajaran Kimia SMA. Skripsi tidak dipublikasikan. Singaraja: Universitas Pendidikan Ganesha, 2010.

Sujiono, S.; Widiyatmoko, A. Pengembangan modul IPA Terpadu berbasis Problem-Based Learning tema gerak untuk meningkatkan kemampuan berpikir kritis siswa. *Unnes Science Education Journal*. **2014**, *3* (3), 685–693. https://doi.org/10.15294/usej.v3i3.4287

Tranfield, D.; Denyer, D.; Smart, P. Towards a methodology for developing evidence-informed management knowledge by means of systematic review. Br. J. Manag. **2003**, *14* (3), 207–222. https://doi.org/10.1111/1467-8551.00375

Utami, T. S.; Santi, D.; Suparman, A. R. Pengaruh Model Pembelajaran Problem-Based Learning (PBL) terhadap Hasil Belajar Kognitif Peserta Didik Kelas XI SMK Negeri 02 Manokwari (Studi Pada Materi Pokok Konsep Laju Reaksi) Tri. *Arfak Chem: Chemistry Education Journal*. **2018**, *1* (1), 21–26. https://doi.org/10.30862/accej.v1i1.45

Yang, L.; Chen, Z.; Liu, T.; Gong, Z.; Yu, Y.; Wang, J. Global Trends of Solid Waste Research from 1997 to 2011 by Using Bibliometric Analysis. *Scientometrics*. **2013**, *96* (1), 133–146. https://doi.org/10.1007/s11192-012-0911-6

Zahrah, F.; Halim, A.; Hasan, M. Penerapan Praktikum dengan Model Problem-Based Learning (PBL) pada Materi Laju Reaksi di Sma Negeri 1 Lembah Selawah. *Indones. J. Sci. Educ.* **2017**, *5* (2), 115–123. https://doi.org/10.24815/jpsi.v5i2.9826

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Variation in the chemical composition of essential oils from *Mangifera indica* L. leaves by comprehensive two-dimensional gas chromatography

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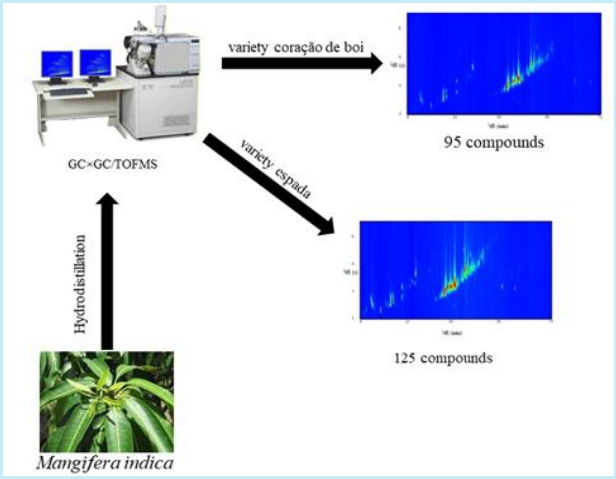
ABSTRACT: The leaves of *Mangifera indica* L. have been used in the medical system of India to treat diseases such as asthma, dysentery, cough, leucorrhea, jaundice, pain, and malaria. The analysis of different varieties of the same species is intended to determine if the compounds have a differential distribution. The present study investigates the volatile compounds from the leaves of two *M. indica* varieties extracted by hydrodistillation and analyzed by comprehensive two-dimensional gas chromatography coupled to time-of-flight mass spectrometry (GC×GC/TOFMS). The number of compounds identified by GC×GC/TOFMS was superior to that obtained by gas chromatography/mass spectrometry (GC/MS) for the same variety of *M. indica*. This study demonstrates the applicability of the GC×GC/TOFMS for the comprehensive profiling of essential oils from *M. indica*, in which 125 and 95 compounds were identified in the varieties 'espada' and 'coração de boi', respectively. These results show that the compositions of the two analyzed essential oils present differences concerning the GC×GC/TOFMS and conventional chromatography technique, the GC/MS.



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1. Introduction

Plant-derived essential oils are known and primarily used for their biological properties (Mesquita *et al.*, 2015). Combined with this, the major interest of the pharmaceutical, food and cosmetics industries in the use of new oils as well as the consumer receptivity to new products of natural origin, transformed the evaluation methods of these plants into widely used tools in the search for new products (Aćimović *et al.*, 2022).

The proportion of individual compounds in the oil composition differs from trace levels to over 90% (Bassolé and Juliani, 2012). Then, the complete separation and the correct identification of the essential oil compounds appear to be very important to a better understanding of the mechanisms involved in those biological activities and the prospection of new active compounds (Cagliero *et al.*, 2022).

Mangifera indica L., belonging to the Anarcadiaceae family, is one of the 40 species of the *Mangifera* genus that can be found in tropical and subtropical regions of Southeastern Asia, Africa, and Latin America (Nikhal and Mahajan, 2010). Its fruits are considered multifunctional foods. However, other parts of this plant, such as bark, flowers, branches, and leaves, have also bioactive compounds (Gupta *et al.*, 2022).

The leaves of *M. indica* have been used in the medical system of India to treat diseases such as asthma, dysentery, cough, leucorrhea, jaundice, pain, and malaria (Basha *et al.*, 2011). In Brazil, the leaves are used as analgesic, anti-inflammatory and the treat hepatitis (Oliveira *et al.*, 2022). The study of the aqueous extracts of the bark of a selected variety of *M. indica* resulted in a pharmaceutical formula, commercially named Vimang. The volatile constituents of *M. indica* fruits present a considerable variation in their chemical composition, which has been extensively investigated (Dzamić *et al.*, 2010). The variability of the volatile constituents can be influenced by factors such as the stage of development, variety, and extraction method (Pino *et al.*, 2005).

The essential oils of *M. indica* leaves from Egyptian varieties have antimicrobial activity (Ouf *et al.*, 2021). The latex essential oil of *M. indica* from the 'rosa' and 'espada' varieties showed cytotoxic activity against HL-60 human tumor cells (Ramos *et al.*, 2014). The volatile compounds in *M. indica* were usually obtained by hydrodistillation and analyzed by gas chromatography/mass spectrometry (GC/MS) (Ansari *et al.*, 2000; Berenbaum *et al.*, 1985; Dzamić *et al.*, 2010; Moreno *et al.*, 2010; Oliveira *et al.*, 2017; Pino *et al.*, 2005).

Due to the volatility and polarity of essential oils components, capillary gas chromatography is the preferable technique for their analysis because essential oils are generally complex mixtures of components with similar physicochemical characteristics (Aspromonte *et al.*, 2019; Rubiolo *et al.*, 2010). However, the satisfactory separation of a complex sample requires a higher peak capacity. In this case, comprehensive two-dimensional gas chromatography (GC×GC), a relatively new technique, can be the best alternative (Keppler *et al.*, 2018).

Comprehensive GC×GC, idealized by Liu and Phillips (1991), has since emerged as the most powerful separation technique for analyzing volatile compounds. The satisfactory separation in complex samples, such as some essential oil, requires a higher peak capacity, achieved using GC×GC. In this technique, two independent separation mechanisms are used to resolve the compounds of complex samples within a single analysis, based on applying two GC columns with different stationary phases connected in series, with a transfer device defined as a modulator. The modulator's function is continuously isolating, reconcentrating, and introducing small portions of the first (1D) effluent onto a second column (2D). The time required to complete this process is defined as the modulation period. Each 1D peak is modulated several times, preserving the 1D separation (Adahchour *et al.*, 2008; Stefanuto *et al.*, 2021).

The GC×GC has the advantage of increasing the resolution and sensitivity of the analysis due to the concentration of the sample fraction through the modulation process allowing the detection of compounds in trace levels as well as the separation of related compounds in the second dimension (Baharum *et al.*, 2010). GC×GC is the most powerful separation system now available when combined with mass spectrometry (MS).

The time-of-flight mass spectrometer (TOFMS) can obtain high spectra acquisition rates for the correct peak assignment and quantification in GC×GC. However, its high cost limits its laboratory utilization. Some studies used GC×GC with a time-of-flight mass spectrometry detector (GC×GC/TOFMS) to analyze essential oils (Eyres *et al.*, 2007; Ieri *et al.*, 2019; Jalali *et al.*, 2012; Rubiolo *et al.*, 2010; Wang *et al.*, 2012). The results obtained by these studies showed an important improvement in the characterization of these samples by GC×GC.

In the present study, the volatile compounds of two *M. indica* were analyzed by GC×GC/TOFMS to evaluate the difference between the compounds in the varieties, allowing an adequate selection for medicinal and industrial purposes.

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2. Experimental

2.1 Samples

The leaves of the *M. indica* variety were collected in Campo Grande/MS, Brazil. The 'espada' variety (collected at 20°30'7" S and 54°37'17" W) and the 'coração de boi' variety (20°30'13" S and 54°37'14" W) were identified by Dr. Ronaldo Posella Zaccaro (Centro Universitário Moura Lacerda, Ribeirão Preto/SP, Brazil) and deposited with voucher specimens' numbers CM105 and CM 107, respectively. All the used solvents and reference standards (linear alkanes) were HPLC grade (JT Baker and Sigma Aldrich). The collection was recorded in the SisGen, number AF9B3C3.

2.2 Essential oil

Each essential oil was isolated from a 400 g sample of fresh leaves of *M. indica* by hydrodistillation using a Clevenger-type apparatus. The essential oils were recovered, dried with anhydrous sodium sulfate, transferred to dark vials, and finally stored at –4 °C for further analysis. Before gas chromatographic analysis, the essential oils (1 mg) were diluted in 1 mL n-hexane. The essential oil yield calculated based on fresh leaves was 0.2% for 'coração de boi' and 0.3% for 'espada'.

2.3 Chromatographic analysis

A GC×GC/TOFMS Pegasus-IV system (LECO, St. Joseph, USA) was equipped with a liquid nitrogen quad-jet modulator and CTC Combi Pal autosampler (CTC Analytics, Carrboro, NC, USA). Electron ionization was 70 eV, the mass acquisition was performed in the range of 50 to 550 amu at 100 Hz, and the detector voltage was –1,706 V. The injector, transfer line and detector temperature were maintained at 250 °C. A conventional column set was employed: DB-5 (5% phenyl–95% dimethylpolysiloxane) with 60 m length, an internal diameter of 0.25 mm, and 0.10 μm of film thickness in the first dimension and a DB-17ms (50% phenyl–50% dimethylpolysiloxane) with 2.15 m length, the internal diameter of 0.18 mm and 0.18 μm of film thickness. Both columns were acquired from Agilent Technologies – J&W Scientific (Palo Alto, CA, USA). The temperature program of the first column started at 50 °C for 5 min, heating at 3 °C min^{-1} till 250 °C. The second column temperature was maintained 10 °C above the temperature of the first column. The modulation period was 10 s, and the Hot pulse was 40% of the modulation period. ChromaTOF software version 3.32 was employed for data processing the total ion current chromatogram, including tools such as peak finder and mass spectra deconvolution. Data processing was performed using a signal-to-noise ratio equal to three. The criterium for accepting a detected compound was a minimum of 80% similarity with the library.

Temperature-programmed retention indices (Mota *et al.*, 2013) were calculated using a mixture of linear alkane (C6-C30), which was analyzed under the same conditions as the chromatographic analysis of the samples. The volatile components' identification was based on comparing their mass spectra with those of the database NIST 2.0, the comparison of their retention index and mass spectrum (Adams, 2007) and the interpretation of the mass spectrum.

The results obtained in this study were compared with the data obtained using GC/MS by Oliveira *et al.* (2017).

3. Results and discussion

Some studies show that the main compounds of the essential oils obtained from mango leaves are sesquiterpenes and monoterpenes (Dzamić *et al.*, 2010; Gerbara *et al.*, 2011; Moreno *et al.*, 2010; Pino *et al.*, 2005). These results of this study corroborate the data on the composition of *M. indica* leaves in the 'espada' and 'coração de boi' varieties.

The essential oil from mango contains constituents such as *α*-gurjunene, trans-caryophyllene, *α*-humulene, *α*-selinene, and camphor (Kumar *et al.*, 2021).

Ramos *et al.* (2014) identified 25 compounds in the essential oil of *M. indica* leaves using gas chromatography with flame ionization detection (GC-FID) and GC/MS. Fontenelle *et al.* (2017) studied the essential oil from different *M. indica* leaves by GC/MS, obtaining 20 compounds for the 'Tommy Atkins' variety, 13 for the 'rosa' variety, 6 for the 'muscat' variety and 15 for the 'jasmine' variety. Ouf *et al.* (2021) identified 31 compounds in the 'Alphonso' variety, 33 compounds in the 'Sidik' variety, 29 compounds in the 'waste' variety, 26 compounds in the 'zebda' variety and 31 compounds in the 'fagri-kalan' variety and trans-caryophyllene (8.06–18.88%), *α*-selinene (4.33–16.92%), and *α*-humulene (8.48–25.98%) were found in the higher concentrations. For the 'coração de boi' variety, cyperene, (*E*)-caryophyllene and *α*-humulene are the predominant compounds. Those compounds were also reported to be the most important in the leaves of the 'coquinho' variety by GC/MS analysis (Gerbara *et al.*, 2011).

The study performed by Oliveira *et al.* (2017) identified 23 volatile compounds such as monoterpenes

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and sesquiterpenes from the leaves of *M. indica* 'espada' and 'coração de boi' varieties extracted by hydrodistillation and analyzed by GC/MS. In the essential oil of leaves obtained from the 'espada' variety, the major compounds were *β*-selinene (34.90%), cyperene (22.40%), (*E*)-caryophyllene (16.39%), *α*-humulene (10.84%), terpinolene (2.31%), and *α*-selinene (2.31%), while in 'coração de boi' variety, the major compounds were cyperene (32.62%), (*E*)-caryophyllene (26.91%), *α*-humulene (17.12%), *β*-selinene (5.70%), myrcene (2.80%), and β-phellandrene (2.70%) Oliveira *et al.* (2017).

The 'espada' and 'coração de boi' varieties generated essential oils of leaves with 125 and 95 tentatively identified compounds using the GC×GC/TOFMS technique. Due to its superior performance over the GC/MS, the GC×GC/TOFMS increased the number of identified peaks in *M. indica* essential oils.

In the column setup used, nonpolar in the 1D and medium polar in the 2D, the compounds are separated in the first dimension based on their different volatilities. In the second dimension, the separation is governed by polarity. Consequently, compounds with similar volatility had similar or even exact retention times in the 1D and will be resolved in the 2D. The GC×GC/TOFMS analyses revealed a complex organic compound mixture (Figs. 1 and 2). Combining a low polar 5% phenyl phase in the first dimension with a medium polar 50% phenyl phase in the second dimension allowed efficient use of the available chromatographic space. Figures 1 and 2 highlight the complexity of the *M. indica* essential oil and the efficiency of GC×GC to reduce the peak coelution, obtaining pure MS spectra and increasing peak detectability.

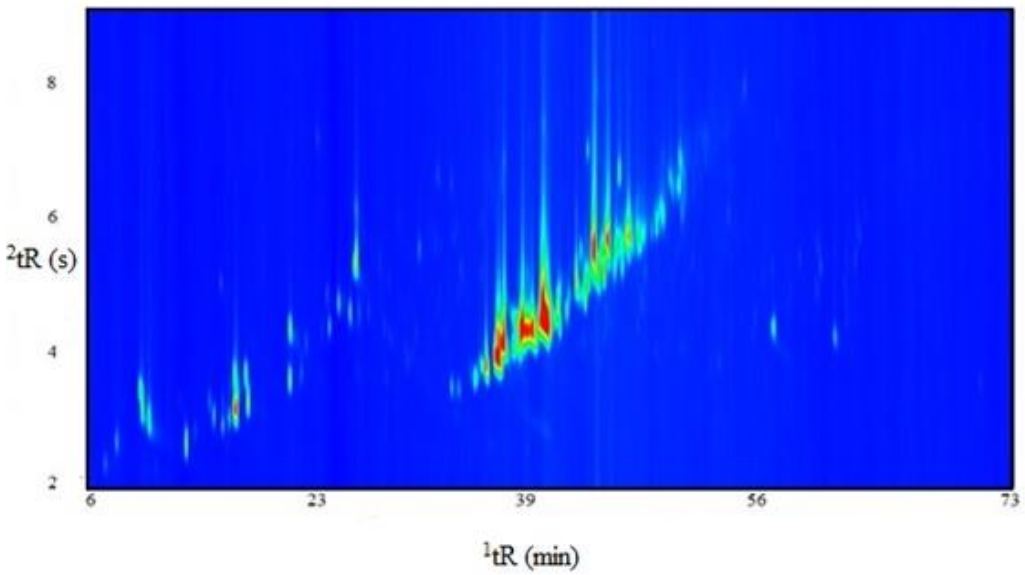

Figure 1. Color diagram of the essential oils of *M. indica* 'espada' variety obtained by comprehensive two-dimensional gas chromatography with time-of-flight mass spectrometric detector.

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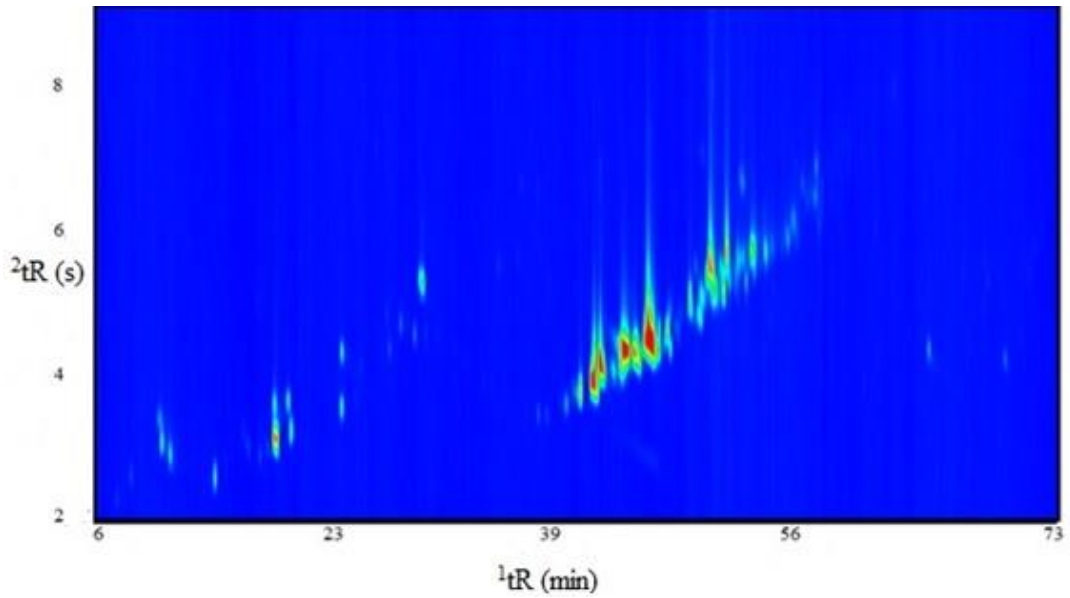

Figure 2. Color diagram of the essential oils of *M. indica* 'coração de boi' variety obtained by comprehensive two-dimensional gas chromatography with time-of-flight mass spectrometric detector.

The experimental linear retention indices show a good agreement between the identified compounds and the linear retention indices reported by literature for 1D-GC (Bogusz Junior *et al.*, 2011). The list of identified compounds is shown in Table 1.

Table 1. Percentage composition of essential oils of leaves of *M. indica* by GC×GC/TOFMS.

KI[a]	KI[b]	^{1}tR	^{2}tR	Compound	'Espada' (%)	'Coração de boi' (%)
769	771	7.83	3.29	2-pentenol	0.05 ± 0.01	-
800	800	8.50	2.02	octane	0.03 ± 0.01	0.05 ± 0.01
800	802	8.50	3.54	caproaldehyde	0.16 ± 0.01	0.16 ± 0.01
848	854	10.17	4.3	2-hexenal	2.10 ± 0.10	1.00 ± 0.10
852	851	10.33	3.97	3-hexen-1-ol	0.44 ± 0.02	0.40 ± 0.03
867	867	10.83	3.85	hexen-1-ol	0.86 ± 0.03	0.81 ± 0.09
867	869	10.83	3.79	santene	1.75 ± 0.09	1.50 ± 0.20
904	902	12.17	4.11	heptanal	0.10 ± 0.01	-
929	930	13.33	3.93	*α*-thujene	0.06 ± 0.01	0.10 ± 0.01
932	939	13.50	3.5	*α*-pinene	1.20 ± 0.10	1.01 ± 0.07
946	944	14.17	2.71	valeric acid 3-methyl	0.07 ± 0.01	-
975	975	15.50	3.91	sabinene	0.30 ± 0.01	0.34 ± 0.01
989	991	16.17	3.79	myrcene	0.21 ± 0.01	1.60 ± 0.10
1000	1000	16.67	3.89	*m*- mentha-1(7).8-diene	0.21 ± 0.01	0.22 ± 0.01
1006	1005	17.00	4.51	*α*- phellandrene	0.33 ± 0.01	0.23 ± 0.01
1010	1011	17.17	4.01	*γ*-carene	4.20 ± 0.10	2.70 ± 0.20
1027	1031	18.00	4.14	limonene	0.99 ± 0.05	1.04 ± 0.08
1033	1031	18.33	5.01	*β*-phellandrene	0.02 ± 0.01	2.80 ± 0.20
1087	1087	21.00	5.22	terpinolene	0.02 ± 0.01	-
1093	1089	21.30	3.21	p-cimenene	0.05 ± 0.01	0.04 ± 0.01
1110	1108	22.17	5.03	maltrol	0.09 ± 0.01	-
1128	1128	23.00	8.03	allo-ocimene	0.09 ± 0.01	-
1134	1134	23.33	5.22	1-terpineol	0.03 ± 0.01	-
1141	1141	23.67	5.73	cis-verbeneol	0.12 ± 0.01	0.22 ± 0.01
1159	1159	24.50	5.61	karahanaenone	0.41 ± 0.03	0.38 ± 0.02
1176	1177	25.33	5.45	terpinen-4-ol	0.35 ± 0.02	0.37 ± 0.01

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1186	1183	25.83	6.15	p-cimen-8-ol	2.00 ± 0.20	2.90 ± 0.20
1190	1190	26.00	3.36	neo isoverbenol	0.25 ± 0.01	-
1211	1212	27.00	3.21	2.4-nonadienal	0.25 ± 0.01	-
1278	1278	30.00	3.27	isopulegyl acetate	0.30 ± 0.01	-
1300	1300	31.00	3.42	tridecane	0.33 ± 0.02	-
1331	1330	32.50	4.85	acetate cis-piperitol	0.02 ± 0.01	-
1334	1333	32.67	7.38	hexyl tiglate	0.08 ± 0.01	0.40 ± 0.02
1338	1339	32.83	6.59	γ-elemene	0.04 ± 0.01	-
1345	1344	33.17	5.77	verbenol acetate	0.08 ± 0.01	0.17 ± 0.01
1348	1348	33.33	6.12	7-epi -silphiperfol-5-one	0.05 ± 0.01	-
1369	1368	34.33	4.51	cyclosativene	0.42± 0.02	0.42± 0.02
1372	1373	34.50	3.36	isoledene	0.39± 0.01	0.58± 0.02
1376	1376	34.67	4.73	α-copaene	0.02 ± 0.01	0.04 ± 0.01
1379	1379	34.83	6.02	silpheperfol-6-one	0.02 ± 0.01	-
1379	1379	34.83	6.85	methyl cinnamate	0.02 ± 0.01	-
1386	1391	35.17	4.67	β-elemene	2.10 ± 0.20	3.10 ± 0.20
1393	1393	35.50	3.55	jasmone	0.35 ± 0.01	0.47 ± 0.02
1397	1398	35.67	4.53	cyperene	5.00 ± 0.30	7.00 ± 0.30
1405	1404	36.01	4.75	methyl eugenol	0.84 ± 0.04	0.84 ± 0.02
1405	1406	36.01	4.85	italicene	3.50 ± 0.30	2.50 ± 0.10
1409	1409	36.17	5.89	α-gurjunene	0.02 ± 0.01	-
1414	1417	36.33	6.61	4.8-alpha-epoxy caryophyllane	0.02 ± 0.01	-
1414	1417	36.33	5.22	sesquitujene	0.02 ± 0.01	-
1414	1418	36.33	5.10	(*e*)-caryophyllene	5.20 ± 0.20	6.50 ± 0.30
1423	1423	36.67	5.69	β-duprezianene	0.06 ± 0.01	0.06 ± 0.01
1427	1429	36.83	4.81	cis thujopsene	0.06 ± 0.01	0.05 ± 0.01
1436	1432	37.17	4.95	β-gurjunene	0.47 ± 0.01	0.52 ± 0.02
1445	1444	37.50	5.30	cedrene	1.04 ± 0.07	1.30 ± 0.10
1450	1450	37.67	4.98	epicedrene	0.13 ± 0.01	0.19 ± 0.01
1450	1450	37.67	5.36	cis-muurola-3.5-diene	0.16 ± 0.01	0.15 ± 0.01
1455	1454	37.83	5.23	α –humulene	6.90 ± 0.30	7.20 ± 0.30
1459	1460	38.00	3.46	β-santalene	0.03 ± 0.01	0.02 ± 0.01
1459	1460	38.00	5.23	allo-aromadendrene	2.10 ± 0.20	2.00 ± 0.10
1473	1473	38.50	5.40	α -terpinyl isobutanoate	0.57 ± 0.02	0.50 ± 0.02
1473	1473	38.50	5.22	drima-7.9(11)-diene	4.80 ± 0.20	4.90 ± 0.20
1477	1477	38.67	5.06	β-gurjunene	0.48 ± 0.02	0.45 ± 0.01
1482	1480	38.83	5.25	γ-murolene	0.30 ± 0.01	0.32 ± 0.01
1486	1480	39.00	5.48	germacrene d	0.72 ± 0.02	0.64 ± 0.02
1486	1485	39.00	5.40	β-selinene	10.20 ± 0.20	10.40 ± 0.20
1495	1496	39.33	3.71	asaricinae	0.28 ± 0.01	0.25 ± 0.01
1495	1498	39.33	5.38	α-selinene	6.70 ± 0.10	5.00 ± 0.20
1500	1500	39.50	5.42	biciclogermacrene	0.87 ± 0.01	0.87 ± 0.03
1509	1509	39.83	5.39	farenol	0.22 ± 0.01	0.21 ± 0.01
1509	1509	39.83	5.24	germacrene a	0.60 ± 0.02	0.62 ± 0.01
1517	1518	40.17	5.34	menthyl isovalerate	0.24 ± 0.01	0.24 ± 0.01
1522	1523	40.33	5.51	eugenol acetate	0.85 ± 0.03	0.83 ± 0.02
1526	1526	40.50	5.80	1-phenyl heptan-3-one	0.18 ± 0.01	0.19 ± 0.01
1526	1527	40.50	5.26	vanillin acetate	0.21 ± 0.01	0.21 ± 0.01
1535	1535	40.83	5.58	10-epi-cubenol	0.33 ± 0.01	0.36 ± 0.02
1539	1539	41.00	5.40	α-cadinene	0.13 ± 0.01	0.17 ± 0.01
1543	1543	41.17	5.75	8.14-cedranoxide	0.43 ± 0.02	0.41 ± 0.01
1548	1548	41.33	6.14	silphiperfolan-6-beta-ol	0.02 ± 0.01	-
1557	1557	41.67	6.93	elemicine	0.03 ± 0.01	0.01 ± 0.01
1561	1561	41.83	5.91	germacrene b	1.31 ± 0.08	2.01 ± 0.12

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1565	1566	42.00	6.32	*β*-calacorene	0.03 ± 0.01	0.03 ± 0.01
1565	1566	42.00	6.42	davanone b	0.23 ± 0.01	0.32 ± 0.01
1574	1575	42.33	5.67	*α*-cedrene epoxy	0.28 ± 0.01	0.25 ± 0.01
1574	1575	42.33	6.01	silphiperfol-5-em-3-one a	0.38 ± 0.01	0.35 ± 0.01
1583	1583	42.67	6.26	turmerol	0.75 ± 0.06	0.34 ± 0.01
1583	1583	42.67	6.43	caryophyllene oxide	3.95 ± 0.08	2.15 ± 0.06
1591	1591	43.00	6.36	*β*-copaen-4-α-ol	0.14 ± 0.01	0.19 ± 0.01
1596	1596	43.17	6.04	turmerone-ar-dihydro	0.60 ± 0.01	0.64 ± 0.02
1600	1600	43.33	3.69	hexadecane	0.01 ± 0.01	-
1600	1601	43.33	5.15	cedrol	0.02 ± 0.01	-
1600	1601	43.33	5.92	guaiacol	0.04 ± 0.01	0.04 ± 0.01
1600	1601	43.33	6.25	*β*-elemenone	0.05 ± 0.01	0.05 ± 0.01
1605	1605	43.50	6.40	sesquilavandulol	0.88 ± 0.03	0.94 ± 0.03
1609	1608	43.67	6.21	platyphyllol	0.17 ± 0.01	0.15 ± 0.01
1609	1608	43.67	6.06	*β*-atlantol	0.92 ± 0.03	1.12 ± 0.05
1614	1614	43.83	6.42	ethyl chromone 2	0.44 ± 0.02	0.40 ± 0.01
1614	1614	43.83	6.59	*β*- biotol	3.40 ± 0.10	4.00 ± 0.20
1618	1618	44.00	6.16	butyl anthranilate	0.12 ± 0.01	-
1632	1631	44.50	6.31	eremoligenol	0.23 ± 0.01	0.27 ± 0.01
1632	1632	44.50	6.55	*γ*-eudesmol	0.82 ± 0.04	0.89 ± 0.02
1641	1641	44.83	7.52	epoxy allo alloaromadendrene	0.34 ± 0.01	0.31 ± 0.01
1645	1646	45.00	6.15	*α*-murolol	0.16 ± 0.01	0.13 ± 0.01
1655	1655	45.33	6.55	dihydromyrcene. 1.6 –diol. e	0.14 ± 0.01	0.15 ± 0.01
1655	1655	45.33	6.61	3- tujopsanone	1.64 ± 0.08	1.4 ± 0.1
1659	1659	45.50	6.62	atractilone	0.61 ± 0.02	0.63 ± 0.03
1668	1668	45.83	6.46	citronellyl tiglate e	0.15 ± 0.01	0.12 ± 0.01
1677	1677	46.17	6.6	cadelene	1.04 ± 0.06	0.90 ± 0.10
1686	1686	46.50	6.65	*α*-bisabolol	0.15 ± 0.01	0.13 ± 0.01
1695	1694	46.83	3.7	germacrone	0.20 ± 0.01	0.22 ± 0.01
1700	1700	47.00	3.79	heptadecane	0.41 ± 0.01	0.43 ± 0.02
1705	1705	47.17	6.68	*δ*-dodecalactone	0.11 ± 0.01	0.14 ± 0.01
1714	1714	47.50	4.91	cedroxide	0.03 ± 0.01	-
1714	1714	47.50	6.76	*α* -humulene. 14hydrixy	0.43 ± 0.01	0.52 ± 0.03
1724	1723	47.83	7.03	crisolide	0.44 ± 0.02	0.48 ± 0.03
1738	1740	48.33	7.53	oplopanone	0.29 ± 0.01	0.34 ± 0.01
1748	1748	48.67	7.29	*α*- oxobisabolone	0.20 ± 0.01	-
1800	1800	50.50	3.85	octadecane	0.23 ± 0.01	0.31 ± 0.01
1897	1898	53.83	4.70	seseline	0.26 ± 0.01	-
1901	1902	54.00	3.91	laurencene	0.26 ± 0.01	-
1963	1962	55.83	5.25	tetrahydro rimuene	1.40 ± 0.10	0.75 ± 0.03
2000	2000	57.00	3.94	eicosane	0.34 ± 0.01	-
2088	2088	59.33	6.16	abietadiene	0.56 ± 0.02	-
2100	2100	60.00	4.03	heneicosane	0.35 ± 0.01	-
2115	2116	60.67	5.14	laurensen-2-one	0.64 ± 0.02	0.73 ± 0.03
2176	2175	62.17	6.63	grandiflorene	0.12 ± 0.01	-

[a]KI: retention index calculated; [b]KI: retention index literature from Adams (2007); (-): not identified; [1]tR: retention time in the first dimension; [2]tR: retention time in the second dimension.

Furthermore, the GC×GC increased the detectability of the compounds due to using the modulator (Baharum *et al.*, 2010), as can be observed in the increase in the number of compounds. These peaks were present at low concentrations, but the improvement of their signal by GC×GC achieved better mass spectra and separation than in the 1D-GC. In several cases, it was found that, despite using two chromatographic separation columns, some compounds were still coeluting. The essential oils have many isomers with similar retention times and mass spectra, especially sesquiterpenes and oxygenated sesquiterpenes. However, peak deconvolution algorithms allowed for resolving chromatographic solutions and extracting the mass spectrum of each

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compound, even in such situations. GC×GC promoted the identification of fivefold more compounds in the two essential oils than GC/MS.

The major constituents of 'espada' variety essential oil identified by GC×GC/TOFMS were β-selinene (10.2%), *α*-humulene (6.9%), *α*-selinene (6.7%), (*E*)-caryophyllene (5.2%), ciperene (5.0%), Drima-7.9(11)-diene (4.8%), γ-carene (4.2%), caryophyllene oxide (3.95%), italicene (3.5%) and *β*-biotol (3.4%). Ninety-five compounds were identified in essential oil of the 'coração de boi' variety by GC×GC/TOFMS and the major constituents were *β*-selinene (10.4%), *α*-humulene (7.2%), ciperene (7.0%), (*E*)-caryophyllene (6.5%), *α*-selinene (5.0%), Drima-7.9(11)-diene (4.9%, *β*-biotol (4.0%) and *β*-elemene (3.1%). A total of 31 compounds were identified exclusively in the 'espada' variety. The two essential oils were characterized by the predominance of *β*-selinene, (*E*)-caryophyllene and *α*-humulene. Also, monoterpenes were found in small concentrations in the two oils.

The use of GC×GC provided enhanced efficiency, mainly for minor compounds. The results showed a considerable increase in the number of separated compounds. In addition, the analysis of mass spectra data together with the retention index allowed the identification of three times more compounds which reflected a differentiation between the essential oils studied.

4. Conclusions

This study demonstrates the applicability of the GC×GC/TOFMS for the comprehensive profiling of *M. indica* essential oils. It also indicated that two-dimensional gas chromatography had a superior resolution, making it possible to identify more compounds. One hundred and twenty-five and ninety-five compounds were tentatively identified in the two studied essential oils of the 'espada' and 'coração de boi' varieties, respectively. These results showed that the compositions of the two analyzed essential oils showed differences in relation to the GC×GC/TOFMS and conventional chromatography technique, the GC/MS.

Authors' contribution

Conceptualization: Cardoso, C. A. L.;
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Formal Analysis: Cardoso, C. A. L.; Castro, T. L. A.;
Funding acquisition: Cardoso, C. A. L.;
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Methodology: Cardoso, C. A. L.; Caramão, E.;
Project administration: Cardoso, C. A. L.;
Resources: Cardoso, C. A. L.;
Software: Cardoso, C. A. L.;
Supervision: Cardoso, C. A. L.; Caramão, E.;
Validation: Cardoso, C. A. L., Simionatto, E.;
Visualization: Cardoso, C. A. L.;
Writing – original draft: Cardoso, C. A. L.; Simionatto, E.; Caramão, E.;
Writing – review & editing: Cardoso, C. A. L.; Castro, T. L. A.

Data availability statement

All data sets were generated or analyzed in the current study.

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References

Aćimović, M.; Rat, M.; Pezo, L.; Lončar, B.; Pezo, M.; Miljković, A.; Lazarević, J. Biological and chemical diversity of *Angelica archangelica* L.—Case study of essential oil and its biological activity. *Agronomy.* **2022**, *12* (7), 1570. https://doi.org/10.3390/agronomy12071570

Adahchour, M.; Beens, J.; Brinkman, U. A. Recent developments in the application of comprehensive two-dimensional gas chromatography. *J. Chromatogr. A.* **2008**, *1186* (1–2), 67–108. https://doi.org/10.1016/j.chroma.2008.01.002

Adams, R. P. *Identification of essential oil components by gas chromatography/mass spectrometry*. Allured Publishing corporation, Illionois, 2007.

Ansari, S. H.; Ali, M.; Neguruel, A. V. J. Isolation and characterization of volatile constituents of mango (*Mangifera indica* cv Safeda) fruits. *Med. Aromat. Plant Sci*. **2000**, *22*, 582–585.

Aspromonte, J.; Wolfs, K.; Adams, E. Current application and potential use of GC × GC in the pharmaceutical and biomedical field. *J. Pharm. Biomed.* **2022**, *176*, 112817. https://doi.org/10.1016/j.jpba.2019.112817

Eclética Química, vol. 48, n. 4, 2023, 27-36
ISSN: 1678-4618
DOI: 10.26850/1678-4618eqj.v48.4.2023.p27-36

Baharum, S. N.; Bunawan, H.; Ghani, M. A.; Mustapha, W. A.; Noor, N. M. Analysis of the chemical composition of the essential oil of polygonum minus huds. using two-dimensional gas chromatography-time-of-flight mass spectrometry (GC-TOF MS). *Molecules.* **2010**, *15* (10), 7006–7015. https://doi.org/10.3390/molecules15107006

Basha, D. P.; Kuman, K. P.; Teja, B. B.; Subbarao, M. Antidiabetic activity on extracts of *Mangifera indica* in alloxan monohydrate induced diabetic rats. *Drug Discov. Today.* **2011**, *3* (7), 165–168.

Bassolé, I. H. N.; Juliani, H. R. Essential oils in combination and their antimicrobial properties. *Molecules* **2012**, *17* (4), 3989–4006. https://doi.org/10.3390/molecules17043989

Berenbaum, M.; Neal, J. J. J. Synergism between myristicin and xanthotoxin, a naturally cooccurring plant toxicant. *Chem. Ecol.* **1985**, *11*, 1349–1358. https://doi.org/10.1007/BF01012136

Bogusz Junior, S.; Melo, A. M. T.; Zini, C. A.; Godoy, H. T. Optimization of the extraction conditions of the volatile compounds from chili peppers by headspace solid phase micro-extraction. *J. Chromatogr.* **2011**, *1218* (21), 3345–3350. https://doi.org/10.1016/j.chroma.2010.12.060

Cagliero, C.; Bicchi, C.; Marengo, A.; Rubiolo, P.; Sgorbini, B. Gas chromatography of essential oil: State-of-the-art, recent advances, and perspectives. *J. Sep. Sci.* **2022**, *45* (1), 94–112. https://doi.org/10.1002/jssc.202100681

Dzamić, A. M.; Marin, P. D.; Gbolade, A. A.; Ristić, M. S. Chemical Composition of *Mangifera indica* Essential Oil from Nigeria. *J. Essent. Oil Res.* 2010, *22* (2), 123–125. https://doi.org/10.1080/10412905.2010.9700279

Eyres, G. T.; Marriott, P. J.; Dufour, J.-P. Comparison of odor-active compounds in the spicy fraction of hop (*Humulus lupulus* L.) essential oil from four different varieties. *J. Agric. Food Chem.* **2007**, *55* (15), 6252–6261. https://doi.org/10.1021/jf070739t

Fontenelle, R. O. S.; Sobrinho, A. C. N.; Soares, B. V.; Aguiar, F. L. L.; Brito, E. H. S.; Cavalcante, C. S. P.; Rocha, M. F. G.; Morais, S. M. Effect of essential oils from *Mangifera indica* L. cultivars on the antifungal susceptibility of *Candida spp.* strains isolated from dogs. *Rev. Bras. Saúde Prod. Anim.* **2017**, *18* (2), 337–346. https://doi.org/10.1590/s1519-99402017000200012

Gerbara, S. S.; Ferreira, W. O.; Ré-Poppi, N.; Simionatto, E.; Carasek, E. Volatile compounds of leaves and fruits of *Mangifera indica* var. coquinho (Anacardiaceae) obtained using solid phase microextraction and hydrodistillation. *Food Chem.* **2011**, *127* (2), 689–693. https://doi.org/10.1016/j.foodchem.2010.12.123

Gupta, A. K.; Gurjar, P. S.; Beer, K.; Pongener, A.; Ravi, S. C.; Singh, S.; Verma, A.; Singh, A.; Thakur, M.; Tripathy, S.; Verma, D. K. A review on valorization of different byproducts of mango (*Mangifera indica* L.) for functional food and human health. *Food Biosci.* **2022**, *48*, 101783. https://doi.org/10.1016/j.fbio.2022.101783

Ieri, F.; Cecchi, L.; Giannini, E.; Clemente, C.; Romani, A. GC-MS and HS-SPME-GC×GC-TOFMS determination of the volatile composition of essential oils and hydrosols (by-products) from Four *Eucalyptus* species cultivated in Tuscany. *Molecules.* **2019**, *24* (2), e226. https://doi.org/10.3390/molecules24020226

Jalali, H. T.; Petronilho, S.; Villaverde, J. J.; Coimbra, M. A.; Domingues, M. R.M.; Ebrahimian, Z. J.; Silvestre, A. J. D.; Rocha, S. M. Deeper insight into the monoterpenic composition of *Ferula gummosa* oleo-gum-resin from Iran. *Ind. Crop. Prod.* **2012**, *36* (1), 500–507. https://doi.org/10.1016/j.indcrop.2011.11.001

Keppler, E. A. H.; Jenkins, C. L.; Davis, T. J.; Bean, H. D. Advances in the application of comprehensive two-dimensional gas chromatography in metabolomics. *TrAC Trends Analyt. Chem.* **2018**, *109*, 275–286. https://doi.org/10.1016/j.trac.2018.10.015

Kumar, M.; Saurabh, V.; Tomar, M.; Hasan, M.; Changan, S.; Sasi, M.; Maheshwari, C.; Prajapati, U.; Singh, S.; Prajapat, R. K.; Dhumal, S.; Punia, S.; Amarowicz, R.; Mekhemar, M. Mango (*Mangifera indica* L.) leaves: Nutritional composition, phytochemical profile, and health-promoting bioactivities. *Antioxidants.* **2021**, *10* (2), 299. https://doi.org/10.3390/antiox10020299

Mesquita, J. M. O.; Cavaleiro, C.; Cunha, A. P.; Lombardi, J. A.; Oliveira, A. B. Estudo comparativo dos óleos voláteis de algumas espécies de Piperaceae. *Rev. Bras. Farmacogn.* **2005**, *15* (1), 6–12. https://doi.org/10.1590/S0102-695X2005000100003

Moreno, A.; Leon, D. F.; Giraldo, G. A.; Rios, E. Análisis del perfil de compuestos volátiles del mango (*Mangifera indica* l. var. Tommy Atkins) tratado por

Eclética Química, vol. 48, n. 4, 2023, 27-36
ISSN: 1678-4618
DOI: 10.26850/1678-4618eqj.v48.4.2023.p27-36

métodos combinados. *Rev. Colomb. Quim.* **2010**, *39* (1), 61–72.

Mota, J. S.; Souza, D. S.; Boone, C. V.; Cardoso, C. A. L.; Caramão, E. B. Identification of the volatile compounds of leaf, flower, root and stem oils of *Piper amalago* (Piperaceae). *J. Essent. Oil Bear. Plants.* **2013**, *16* (1), 11–16. https://doi.org/10.1080/0972060X.2013.794021

Nikhal, S.; Mahajan, S. D. J. Evaluation of antibacterial and antioxidant activity of *Mangifera indica* (leaves). *J. Pharm. Sci. Res.* **2010**, *2* (1), 45–47.

Oliveira, R. M.; Dutra, T. S.; Simionatto, E.; Kassuya, C. A. L.; Cardoso, C. A. L. Anti-inflammatory effects of essential oils from *Mangifera indica*. *Genet. Mol. Res.* **2017**, *16* (1), gmr16019227. https://doi.org/10.4238/gmr16019227

Oliveira, Y. R.; Sousa, W. G. M.; Silva, P. H.; Pacheco, A. C. L.; Abreu, M. C. Anacardiaceae na medicina tradicional de comunidades rurais do Piauí, nordeste do Brasil. *Ensaios Ciênc.* **2022**, *26* (1), 32–42. https://doi.org/10.17921/1415-6938.2022v26n1p32-42

Ouf, S. A.; Galal, A. M. F.; Ibrahim, H. S.; Hassan, A. Z.; Mekhael, M. K. G.; El-Yasergy, K. F.; El-Ghany, M. N. A.; Rizk, M. A.; Hanna, A. G. Phytochemical and antimicrobial investigation of the leaves of five Egyptian mango cultivars and evaluation of their essential oils as preservatives materials. *J. Food Sci. Technol.* **2021**, *58* (8), 3130–3142. https://doi.org/10.1007/s13197-020-04816-5

Liu, Z. Y.; Phillips, J. J. Comprehensive two-dimensional gas chromatography using an on-column thermal modulator interface. *Chromatogr. Sci.* **1991**, *29* (6), 227–231. https://doi.org/10.1093/chromsci/29.6.227

Pino, J. A.; Mesa, J.; Munoz, Y.; Martia, M. P.; Marbot, R. J. Volatile Components from Mango (*Mangifera indica* L.) Cultivars. *Agric. Food Chem.* **2005**, *53* (6), 2213–2223. https://doi.org/10.1021/jf0402633

Ramos E. H. S.; Moraes, M. M.; Nerys, L. L. A.; Nascimento, S. C.; Militão, G. C. G.; Figueiredo, R. C. B. Q.; Câmara, C. A. G.; Silva, T. G. Chemical composition, leishmanicidal and cytotoxic activities of the essential oils from *Mangifera indica* L. var. rosa and espada. *BioMed Res. Int.* **2014**, *2014*, 734946. https://doi.org/10.1155/2014/734946

Rubiolo, P.; Sgorbini, B.; Liberto, E.; Cordero, C.; Bicchi, C. J. Essential oils and volatiles: Sample preparation and analysis. A review. *Flavour Fragr.* **2010**, *25* (5), 282–290. https://doi.org/10.1002/ffj.1984

Stefanuto, P.-H.; Smolinska, A.; Focant, J.-F. Advanced chemometric and data handling tools for GCxGC-TOF-MS: Application of chemometrics and related advanced data handling in chemical separations. *Trends Anal. Chem.* **2021**, *139*, e116251. https://doi.org/10.1016/j.trac.2021.116251

Wang, K.; Zhu, R.-z.; Qu, R.-f.; Li, Z.-y. Comprehensive two-dimensional gas chromatography–time-of-flight mass spectrometry for the analysis of volatile components in Neroli essential oil. *Mendeleev Commun.* **2012**, *22* (1), 45–46. https://doi.org/10.1016/j.mencom.2012.01.018

Eclética Química, vol. 48, n. 4, 2023, 27-36
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Multivariate statistical analysis of physicochemical parameters of groundwater quality using PCA and HCA techniques

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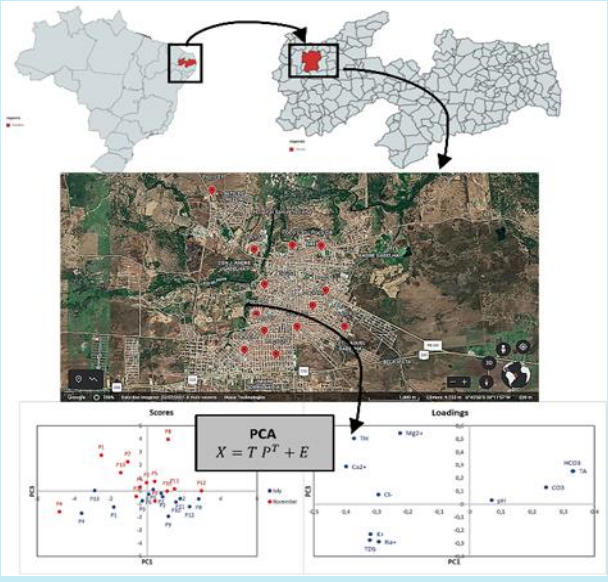
ABSTRACT: Multivariate analysis techniques are powerful tools in the study of groundwater quality, providing an expanded view of quality parameters. This work presents a multivariate analysis of groundwater quality in the city of Sousa, Paraíba state, through the techniques of principal component analysis (PCA) and hierarchical cluster analysis (HCA). Samples from 13 tubular wells were collected in different districts of the city of Sousa, during the rainy and dry seasons. For these samples, 11 parameters were analyzed: hydrogenic potential (pH), total dissolved solids, total alkalinity, carbonates, bicarbonates, total hardness, magnesium, calcium, sodium, potassium, and chlorides. PC1, PC2, PC3 and PC4 explain 87.48% of the total variance of the data. The PCA shows that there was a change in patterns between the analyzed periods. The correlation matrix corroborates the PCA data, showing the relationships between the physical-chemical variables evaluated. The HCA confirmed the correlations between the samples, making it possible to assess the degree of similarity between the composition of the wells and between the parameters evaluated.



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1. Introduction

Water scarcity and poor distribution are the greatest obstacles for the socioeconomic development of the Brazilian semiarid region. According to Rossiter *et al.* (2020), in the northeastern semiarid, water does not have a uniform distribution, neither in time nor in space, and depends on climate vulnerability. The relationship between precipitation and evaporation presents a negative balance, resulting in long periods of drought throughout the year.

In regions with a semiarid climate, well drilling is the main activity to access water, an indispensable resource for life, industry, and agriculture. Deterioration in both quantity and quality of underground water poses a potential threat to urban and rural communities that depend on this resource.

Underground water quality largely depends on hydrochemical processes carried out through regional hydrogeological and anthropogenic activities under saturated and unsaturated soil conditions.

Some human activities that cause inadequate disposal of domestic sewage can significantly compromise the quality of underground water in shallow aquifers, which are quite vulnerable to contamination. Underground waters in urban areas are more susceptible to quality deterioration due to inappropriate use and occupation of the soil, the flow of various effluents discarded in the soil, and seasonality, which affects the recharge of these springs.

The analysis, monitoring and assessment of underground water quality parameters can be used to detect possible contamination events and as an indication of significant changes in physical and chemical properties of water, thereby avoiding financial and social losses. However, the assessment of a single parameter in isolation is not enough to describe the water quality, requiring a larger set of parameters and a multivariate analysis.

In this sense, multivariate statistical analysis techniques can be valuable tools to understand the characteristics and behavior of the aquifer that affect the quality control of underground water.

According to Taşan *et al.* (2022), the use of multivariate statistical methods together with geographic information systems contributes to the efficient management of water resources, planning and decision-making.

Carvalho *et al.* (2015) reported that, in recent years, the use of multivariate statistical methods, such as the principal component analysis (PCA) and hierarchical cluster analysis (HCA), have been frequently applied in numerous studies as a useful chemometric tool to extract a greater number of information obtained through the analysis of physicochemical and microbiological parameters, and metallic elements in samples of surface water, underground water, rain and minerals.

According to Gomes and Cavalcante (2017), by using the PCA technique, it is possible to select the characteristics with the highest participation in each component and define which physical-chemical parameters of the water should be monitored, thus reducing costs with analyses of factors of lesser importance in water quality.

In short, "PCA is an unsupervised pattern recognition method capable of transforming a set of experimental data into informative graphs about the similarity between samples and their respective variables" (Valderrama *et al.*, 2016, p. 245). According to Lyra *et al.* (2010), in this technique, a data matrix called matrix X is decomposed into a product of two other matrices, one called matrix of scores (T) and the other called matrix of loadings (P), such as Eq. 1:

$$X = TP^T + E \quad (1)$$

where P^T represents the transposed loadings matrix and E a residue matrix. The matrix of scores (T) presents information about the samples (rows of X, while the matrix of loadings (P) provides information about the variables (columns of X).

Importantly, several works have been developed in recent years with the purpose of applying exploratory data analysis tools to evaluate the hydrogeochemical characteristics of different water sources, including: Carvalho *et al.* (2015), Pan *et al.* (2019), Nnorom *et al.* (2019), Chaves *et al.* (2020) and Lopes *et al.* (2022).

Carvalho *et al.* (2015) investigated underground water samples from 17 locations distributed in the urban area of Belém, Pará state, Brazil. For all samples, seven physicochemical parameters and nine trace elements were evaluated. The PCA revealed the separation of two distinct groups of samples (A and B), due to the differences presented by the variables total dissolved solids (TDS), electrical conductivity and turbidity among the studied neighborhoods. The combination of principal components (PC) explained 85.7% of the total variance of the data, and PC1 (30.3%) and PC2 (22.4%) were the ones that most contributed to the discrimination of the samples.

Nnorom *et al.* (2019) examined the physicochemical and trace element contents of ground and surface water sources in the shale bedrock terrain of Southeastern Nigeria. A total of 124 water samples were collected from rural areas and analyzed for 21 elements. Different multivariate statistical approaches applied to assess the

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origins of elements in water bodies identified six source types that accounted for 70.88% of the total variance. Anthropogenic activities were considered to contribute much of Cu, Pb, Cd, Cr, Li and P, while Al, As, Co, Fe, Se, Ni, Y and V were likely from crustal materials, minerals and ores, and natural environments. Cluster analysis was adopted to classify 124 sample points into two water pollution groups, reflecting influences from soil materials and anthropogenic sources.

Pan *et al.* (2019) conducted a study on the groundwater quality of the Condie Aquifer in Saskatchewan, Canada, where the Regina landfill was constructed without an engineered liner. An integrated statistical approach using PCA, correlation analysis, ion plots and multiple linear regression was used to evaluate groundwater contamination at the Regina landfill. Correlation analysis and ion plots pointed to gypsum and halite dissolution as the major factors affecting groundwater chemistry. PCA yielded three principal components, responsible for 80.7% of the total variance. A group analysis of the wells suggested possible groundwater contamination from the landfill operation. A two-step multiple linear regression was used to develop a model for predicting total hardness.

Chaves *et al.* (2020) studied the groundwater of 20 locations in Parauapebas, Pará state, Brazil, investigating nine physicochemical parameters in each sample. PCA and HCA revealed significant differences between the samples, being possible to observe the formation of two distinct groups (A and B). The most significant physicochemical parameters for separating the two groups were temperature, pH, electrical conductivity, color, chloride content, and TDS.

Lopes *et al.* (2022) studied the effects of the transfer of the São Francisco River on the performance of the water treatment plant of Gravatá, Paraíba state, Brazil. Using factor analysis combined with PCA (FA/PCA), the authors identified changes in the apparent color and turbidity of raw water, thus requiring interventions in the coagulation/flocculation/decantation processes. Moreover, by monitoring the volume of the Epitácio Pessoa reservoir, from January 2016 to December 2017, PCA and HCA exhibited the distinction of different phases in the water quality of the reservoir.

In this context, the present study aims to perform a multivariate analysis of the physicochemical quality parameters of underground water from tubular wells in the municipality of Sousa, Paraíba state, Brazil, to maximize the amount of information extracted and consequently, better interpret the correlations and similarities between samples and variables.

2. Experimental

The study was conducted in the urban area of the municipality of Sousa, Paraíba state, located in the semiarid zone of Brazilian northeastern region.

Samples from 13 tubular wells were collected from different districts of Sousa, as illustrated in Fig. 1 and described in Table 1, at the end of the rainy season (July) and the dry season (November). Samples were collected at the same time, starting at 7:00 am, and were packed in 500 mL plastic bottles, properly cleaned and sterilized, kept in thermal boxes during transport, cooled to 10 °C. The analyzes were carried out at the Chemistry Laboratory of the Campus Sousa, of the Instituto Federal de Educação, Ciência e Tecnologia da Paraíba.

Some wells drilled by the municipal government, over time, were out of operation, either because their water reserves were empty, or because of problems with the pumping system. As a result, the number of wells in operation during the execution of the study was reduced, limiting the number of wells sampled to 13. The points chosen by the municipal water department for drilling the wells included public areas such as squares, sidewalks, parks, etc. As the city is located on a crystalline subsoil, heterogeneity in both flow and depth in drilled wells is common.

For these samples, 11 physicochemical quality parameters were investigated: hydrogen potential (pH), TDS, total alkalinity (TA), carbonates (CO_3^{2-}), bicarbonates (HCO_3^-), total hardness (TH), magnesium (Mg), calcium (Ca), sodium (Na), potassium (K) and chlorides (Cl). Theses parameters are associated to the geochemical characteristics of the region's subsoil. The methodology used to determine the physicochemical parameters was conducted in accordance with the *Standard Methods for the Examination of Water and Wastewater*, 23 ed. (Baird *et al.*, 2017).

The parameters TA, TH, carbonates (CO_3^{2-}), bicarbonates (HCO_3^-), magnesium (Mg^{2+}), calcium (Ca^{2+}), sodium (Na^+), potassium (K^+) and chlorides (Cl^-) were determined by titration, in triplicate. The pH was measured using a pH meter (model pHB-500, Ion), and the TDS content was obtained using a multiparameter equipment (model Logen, LS).

For the multivariate statistical analysis, PCA, correlation matrix and HCA techniques were used, with the aid of The Unscrambler software, version 9.7, CAMO.

Initially, a data matrix was constructed with 26 lines (referring to the 13 wells sampled at two different times) and 11 columns (referring to the 11 parameters

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evaluated). The first 13 lines refer to the data of the quality parameters at the end of the rainy season (July), and the last 13 lines refer to parameter data in the dry season (November). As a resource for preprocessing of the original data matrices, autoscaling was used. The autoscaling technique was chosen because the values of the evaluated parameters show distributed values in different ranges, and it is necessary that the same weight be assigned to each variable under study.

PCA was used to explore the association between parameters that influence groundwater quality, reducing the number of variables and verifying which variables or sets of variables explain most of the total variability, showing the relationships between them. As a result, two-dimensional plots of scores and loadings are obtained, allowing a better visualization of the distribution of experimental data and the relationships between variables and between samples (Souza and Poppi 2012).

Regarding HCA, its use consists of analyzing a set of data through hierarchically defined groups, verifying the similarity between variables or samples, as a complementary strategy to PCA (Mingoti, 2007). In this study, HCA was applied to the autoscaled data, and the measure of similarity chosen was the squared-Euclidean distance and as a hierarchical clustering criterion, the Single-Linkage method was used, which considers the total sum of deviations of each object in relation to the group mean. From the HCA calculations, the dendrograms of the samples and variables were generated, allowing to identify the degree of similarity between the groups.

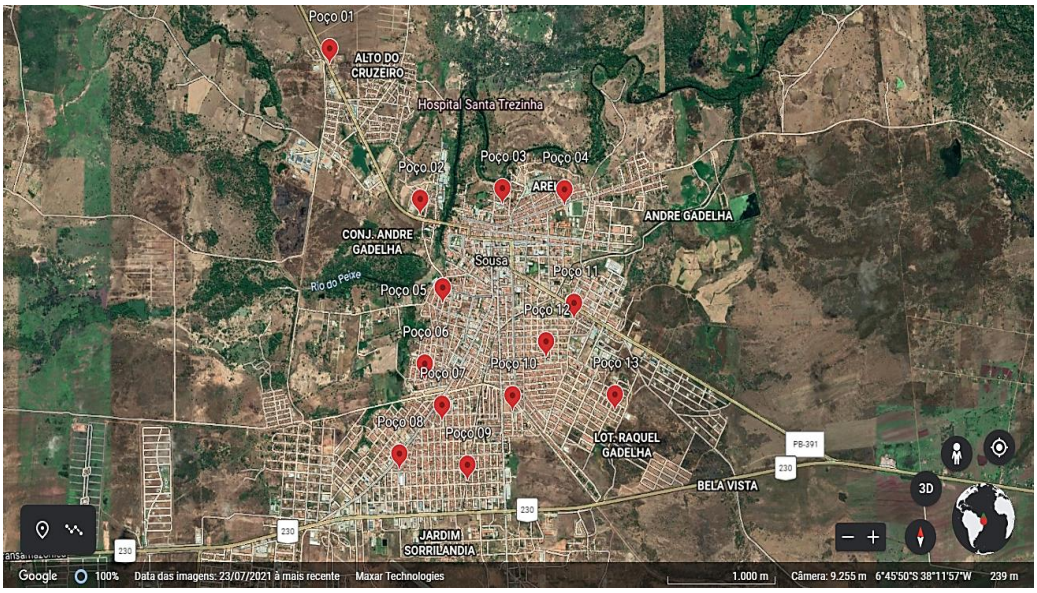

Figure 1. Geolocation of the sampled wells.
Source: Adapted from Google Earth, 2021.

Table 1. Technical information of the sampled wells.

Well	Drilling date	Depth (m)	Flow (l/h)	Location	Localization
01	06/09/2015	51	1,500	Alto do Cruzeiro	–6.74605, –38.24398
02	05/28/2015	50	600	Várzea da Cruz (PSF)	–6.75668, –38.23644
03	05/24/2015	51	2,000	Guanabara (PSF)	–6.75585, –38.2295
04	05/25/2015	51	1,800	Estádio Marizão	–6.75594, –38.22425
05	07/20/2015	41	5,538	Alto Capanema	–6.7632, –38.23455
06	08/08/2015	49	10,000	Jardim Santana	–6.76883, –38.23607
07	05/27/2015	50	600	Estação (PSF)	–6.77187, –38.23461
08	07/24/2015	40	3,130	Jardim Bela Vista (Varejão)	–6.77547, –38.23821
09	06/23/2015	51	1,142	Jardim Sorrilândia II	–6.77631, –38.23246
10	08/18/2015	50	2,300	Casas Populares (CSU)	–6.77116, –38.22865
11	07/20/2015	51	1,400	Condomínio Doca Gadelha	–6.76434, –38.22344
12	06/19/2015	51	700	Conjunto Dr. Zezé	–6.76718, –38.22581
13	06/06/2015	51	5,200	Alto do DNOCS	–6.7711, –38.21999

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3. Results and discussion

The average values of the results corresponding to the 11 physicochemical parameters determined in the 13 examined wells, at the end of the rainy season, are described in Table 2, while data for the dry season are shown in Table 3.

Table 2. Results of physicochemical analysis at the end of the rainy season (July).

	Parameters										
	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)
	TA	CO_3^{2-}	HCO_3^-	TH	Mg^{2+}	Ca^{2+}	Cl^-	Na^+	K^+	pH	TDS
Well 01	129.60	0.52	157.05	171.00	15.75	47.29	493.44	494.70	1.81	7.83	1027.0
Well 02	355.20	1.68	429.92	124.20	21.00	16.83	172.58	212.10	1.77	7.90	490.0
Well 03	276.00	1.80	333.06	144.00	12.68	40.88	397.69	489.60	1.08	8.04	987.0
Well 04	412.80	2.69	498.14	230.40	23.18	60.12	480.23	1781.80	4.10	8.04	2713.0
Well 05	590.40	1.31	717.62	156.60	15.75	40.88	459.22	504.90	2.20	7.57	993.0
Well 06	396.00	1.01	481.06	163.80	15.75	44.09	166.58	159.60	2.60	7.63	453.0
Well 07	508.80	1.42	617.84	136.80	10.94	40.88	282.13	316.20	2.00	7.67	688.0
Well 08	616.80	4.41	743.54	39.60	5.25	8.02	315.15	453.90	1.19	8.08	788.0
Well 09	511.20	4.58	614.34	34.20	2.62	10.42	472.73	1080.70	1.49	8.18	1723.0
Well 10	528.00	1.23	641.66	77.40	7.44	20.84	184.59	337.90	1.96	7.59	613.0
Well 11	626.40	1.92	760.30	73.80	9.19	16.03	342.16	515.10	1.70	7.71	921.0
Well 12	494.40	6.08	590.80	34.20	3.50	8.82	316.65	617.10	1.07	8.32	1038.0
Well 13	376.80	0.86	457.95	243.00	20.12	71.34	997.98	766.80	2.50	7.58	1497.0
Minimum	129.60	0.52	157.05	34.20	2.62	8.02	166.58	159.60	1.07	7.57	453.0
Maximum	626.40	6.08	760.30	243.00	23.18	71.34	997.98	1781.80	4.10	8.32	2713.0
Average	447.88	2.27	541.79	125.31	12.55	32.80	390.86	594.65	1.96	7.86	1071.6
Standard deviation	143.01	1.70	173.09	70.01	6.75	20.69	216.88	429.15	0.81	0.25	612.2

Units: TA and TH (mg $CaCO_3$ L^{-1}); CO_3^{2-}, HCO_3^-, Mg^{2+}, Ca^{2+}, Cl^-, Na^+ and K^+ (mg L^{-1}); pH (unit); TDS (ppm).

Table 3. Results of physicochemical analysis during the dry season (November).

	Parameters										
	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)
	TA	CO_3^{2-}	HCO_3^-	TH	Mg^{2+}	Ca^{2+}	Cl^-	Na^+	K^+	pH	TDS
Well 01	355.20	2.54	428.18	392.40	50.74	81.76	580.78	749.70	1.03	8.08	1073.0
Well 02	388.80	3.18	467.86	212.40	29.74	40.08	220.61	327.60	2.20	8.14	578.2
Well 03	259.20	2.43	311.28	165.60	10.50	54.51	556.02	392.70	1.03	8.20	1000.0
Well 04	259.20	2.27	311.60	273.60	17.50	89.78	675.32	1615.70	3.20	8.17	3162.0
Well 05	648.00	2.87	784.73	181.80	9.19	64.13	589.78	423.30	2.00	7.87	1035.0
Well 06	460.80	0.94	560.27	208.80	3.06	87.37	240.87	136.50	2.50	7.53	461.7
Well 07	494.40	2.09	598.92	322.20	33.68	81.76	366.93	270.30	2.00	7.85	763.6
Well 08	717.60	7.89	859.43	327.60	55.55	44.09	378.18	408.00	0.99	8.27	878.1
Well 09	516.00	6.50	616.31	117.00	7.44	38.48	578.53	949.40	1.50	8.33	1847.0
Well 10	561.60	2.79	679.49	135.00	5.69	49.70	312.90	365.80	1.92	7.92	718.9
Well 11	679.20	3.69	821.12	126.00	0.87	54.51	429.96	515.10	1.57	7.96	1025.0
Well 12	636.00	10.25	755.07	75.60	1.75	30.46	357.92	576.30	0.91	8.44	1070.0
Well 13	566.40	2.87	685.16	255.60	24.06	69.74	1040.00	674.50	1.79	7.93	1367.0
Minimum	259.20	0.94	311.28	75.60	0.87	30.46	220.61	136.50	0.91	7.53	461.7
Maximum	717.60	10.25	859.43	392.40	55.55	89.78	1040.00	1615.70	3.20	8.44	3162.0
Average	503.26	3.87	606.11	214.89	19.21	60.49	486.75	569.61	1.74	8.05	1152.3
Standard deviation	152.49	2.67	183.22	94.72	18.40	20.09	220.19	380.91	0.67	0.24	698.4

Units: TA and TH (mg $CaCO_3$ L^{-1}); CO_3^{2-}, HCO_3^-, Mg^{2+}, Ca^{2+}, Cl^-, Na^+ and K^+ (mg L^{-1}); pH (unit); TDS (ppm).

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Notably, similar values in magnitude were obtained for the physicochemical parameters of groundwater quality by Jiang *et al.* (2015), in Mongolia, Taşan *et al.* (2022), in Turkey, and Chaves *et al.* (2020), in Pará state, Brazil.

The results of the multivariate analysis are hereafter presented. As PCA causes a change in the vector space of the data set, each object (each of the 13 sampled wells) that was represented in a space with 11 variables (11 physicochemical parameters) is represented by 11 principal components. Figure 2 illustrates the variances explained by the first 7 accumulated principal components referring to the data collected in the months of July and November. Since the first principal components are responsible for most of the data variance, it is possible to concentrate the analysis focusing on a smaller number of variables, without a significant loss of information being observed. In this case, the first four principal components explain 87.48% of the total variance, which were chosen because they have eigenvalues greater than 1.0.

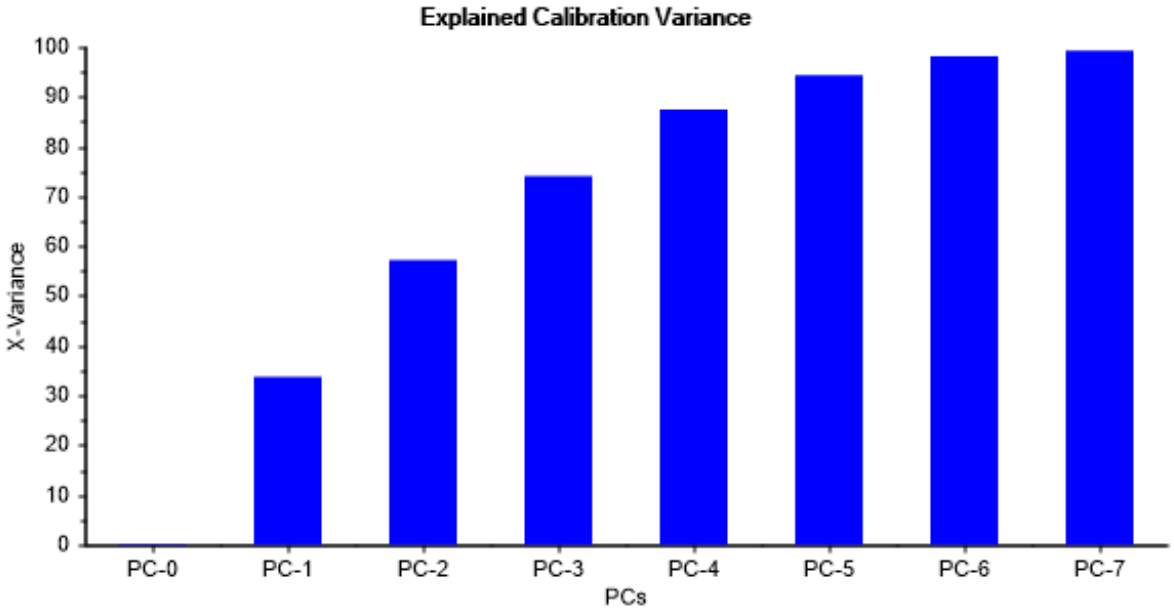

Figure 2. Cumulative variance explained by the principal components.

Figures 3 and 4 show the score and loading plots, respectively, for PC1 and PC3, for the months of July and November. According to Lyra *et al.* (2010), the scores are projections of the original objects in the space of the principal components, that is, they are the new coordinates of the objects in the new variables. In this case, the score plot indicates the relationships between the sampled wells. Furthermore, the authors state that the loadings, or weights, geometrically represent the cosines of the angles that the principal components make with the original variables. In this case, in the loading plot, we can observe the relationships between the variables, that is, between the physicochemical parameters evaluated.

Some important patterns can be noticed in the score plot in Fig. 3. For example, the wells 1, 4 and 13 are located on the negative side of PC1, isolated from the other wells, hence indicating that they differ significantly from the others in terms of their chemical composition. This can be verified in Tables 2 and 3, which reveal the high concentration of salts in these three samples.

Another arrangement of scores that draws considerable attention refers to the wells 2, 3, 5, 6 and 7, which are concentrated in the same region, indicating that these samples have some similarity in their composition. This fact can be associated with the proximity of these wells to the bed of the Rio do Peixe that passes through the urban area of the municipality. This proximity may be promoting a more uniform recharge in these wells in comparison to the others.

It is also visible the pattern changes between the sampled wells in relation to the period of the year in which the analysis was conducted. Figure 3 clearly illustrates that the data from the wells sampled in July, at the end of the rainy season, are concentrated on the negative side of PC3. The data from the wells sampled in November (drought period) are on the positive side of PC3. This finding indicates a substantial change in the composition of groundwater in the studied area in relation to the time of collection in the year. Comparing with the loadings plot in Fig. 4, it can be inferred that the

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data from the analysis for the month of July are concentrated on the negative side of PC3, as well as the variables Na^+, K^+ and TDS. This can be explained because, during the rainy season, there is a greater percolation of water in the soil, causing a greater dissolution of sodium and potassium salts, increasing the concentration of these ions in the water. With respect to the data for the month of November, the scores are concentrated on the positive side of PC3, as well as the parameters related to alkalinity and hardness of the water, which are parameters more related to the rock in which the groundwater is deposited. With the lack of recharge during the dry season, the ions responsible for alkalinity and hardness tend to be concentrated during this period.

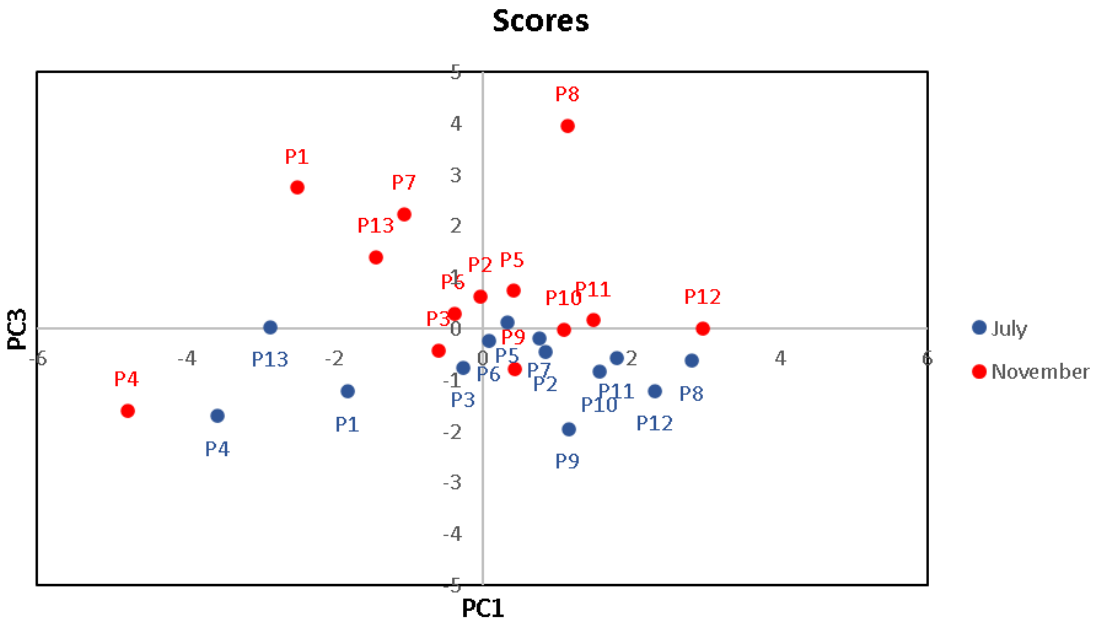

Figure 3. Plot of PCA scores of the wells sampled in July and November.

In the PCA loadings plot (Fig. 4), correlations between variables are easily detected. It is the case of TA, concentrations of carbonate ions (CO_3^{2-}), bicarbonates (HCO_3^-) and pH, indicating that the hydrogenic potential of the water of the wells throughout the year is mainly determined by the content of carbonate and bicarbonate ions, which, due to the basic character, are responsible for the alkalinity, maintaining the pH above 7.0, as recorded in Tables 2 and 3. It is worthwhile noting the close relationship between total alkalinity and bicarbonate ion concentration (HCO_3^-), confirming that most of the alkalinity of these wells is owing to the presence of the HCO_3^- ion.

Another pattern observed is the relationship of similitude between sodium ion and TDS content, indicating that this ion is the main responsible for the high TDS values.

Additionally, the group of variables total hardness, calcium and magnesium are also very close in the loadings plot, thus implying that they are correlated. Indeed, the definition of total hardness is intrinsically associated with the concentrations of divalent metal cations (Harris, 2017).

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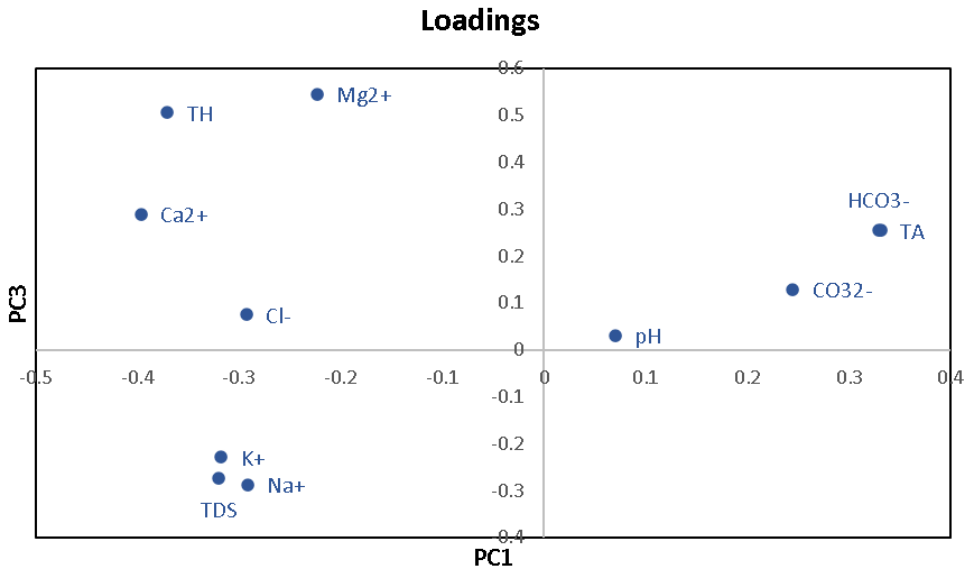

Figure 4. Plot of PCA loadings of physicochemical parameters in the months of July and November.

The correlation coefficient matrix between the physicochemical parameters evaluated is depicted in Table 4. The data from the correlation matrix evidence the similarities between variables presented in the PCA loading plot. There is a very significant correlation between the concentration of bicarbonate ions (HCO_3^-) and TA, reinforcing that this ion is the leading cause of the alkaline character of the samples. There are also strong positive correlations ($r > 0.7$) for the pairs CO_3^{2-} and pH, Na^+ and TDS, corroborating the PCA data.

A strong correlation between the concentrations of calcium (Ca^{2+}) and magnesium (Mg^{2+}) ions with the total hardness was also observed, which agrees with the PCA loading plot, emphasizing that the hardness is caused by the presence of multivalent metallic cations. This correlation also suggests the dissolution of calcite ($CaCO_3$) and dolomite [$CaMg(CO_3)_2$] in these aquifers, the main components of sedimentary rocks (Celestino *et al.*, 2018). Similar findings were reported by Charfi *et al.* (2013).

Table 4. Correlation matrix for the physicochemical parameters evaluated.

	TA	**CO_3^{2-}**	**HCO_3^-**	**TH**	**Mg^{2+}**	**Ca^{2+}**	**Cl^-**	**Na^+**	**K^+**	**pH**	**TDS**
TA	**1**										
CO_3^{2-}	0.5057	**1**									
HCO_3^-	**0.9997**	0.4856	**1**								
TH	–0.2287	–0.1955	–0.2265	**1**							
Mg^{2+}	–0.1171	–0.0066	–0.1185	**0.8397**	**1**						
Ca^{2+}	–0.2665	–0.3260	–0.2613	**0.8222**	0.3813	**1**					
Cl^-	–0.1126	–0.0369	–0.1131	0.3906	0.1721	0.4846	**1**				
Na^+	–0.1816	0.1502	–0.1880	0.1407	0.0463	0.1910	0.4746	**1**			
K^+	–0.2342	–0.4922	–0.2242	0.2553	0.0124	0.4216	0.0960	0.4623	**1**		
pH	0.0383	**0.8060**	0.0172	–0.0621	0.0927	–0.2030	0.0738	0.3757	–0.4316	**1**	
TDS	–0.2125	0.1243	–0.2187	0.1858	0.0214	0.2939	0.5521	**0.9709**	0.4720	0.3589	**1**

The observed results can be explained from the geological aspects of the sedimentary basin of the Rio do Peixe, described by Galvão *et al.* (2005), where the studied area is located, which is constituted by rocks of the Precambrian Crystalline Complex. This group is predominantly made up of clayey rocks (claystones and shales), which resulted in the formation of thin layers of salts in the form of films (mainly Ca^{2+}, Na^+, K^+ associated with HCO_3^- and CO_3^{2-}).

Figure 5 illustrates the dendrogram of the HCA of the data from the wells collected during the dry season. According to Ferreira (2015), the main purpose of HCA is to gather samples in such a way that those belonging to the same group are more similar to each other than to samples from other groups.

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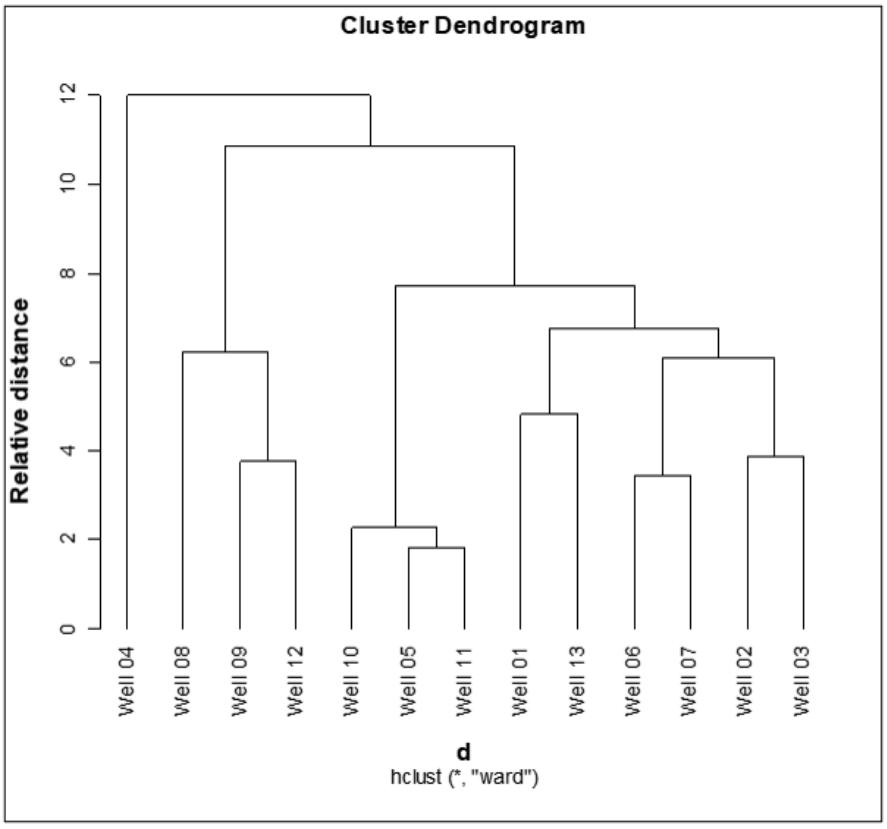

Figure 5. HCA dendrogram of the dry season for the sampled wells.

Figure 5 demonstrates some patterns of similarity between the samples. The wells 05, 11 and 10 present a high degree of similarity, as can be seen from the small relative distance between them in the dendrogram. This result implies that these samples have a uniform composition among themselves, which is corroborated by the PCA scores plot (Fig. 3), in which these wells are very close to each other.

It is also noteworthy the high relative distance of the wells 08 and 04 in relation to the others, suggesting that the waters of these points have a very different composition from the other wells. This result can be confirmed through Fig. 3. In relation to the other samples, from the analysis of the HCA dendrogram, it is verified that they present a certain degree of similarity to each other.

4. Conclusions

The findings of this study revealed that the waters of the tubular wells in the urban area of the municipality of Sousa have high levels of bicarbonate, chloride, and sodium ions, which also increases the values of total alkalinity and TDS, thereby making the consumption of some samples unfeasible, and limiting the use of these waters only for domestic cleaning activities.

PCA showed that there was a change in the patterns between the analyzed periods, July, and November, which proves the influence of the rainy season on the recharge and water composition of these wells. The first four principal components explain 87.48% of the total variance of the data. PCA also demonstrated that some parameters are well correlated, such as alkalinity, pH, HCO_3^- and CO_3^{2-}; total hardness, Ca^{2+} and Mg^{2+}; TDS, Na^+ and K^+. The correlation matrix corroborates the PCA data, showing the relationships between the physicochemical variables evaluated. HCA confirmed the correlations between the samples, thus allowing to assess the degree of similarity between the composition of the wells and between the parameters evaluated. From the HCA, it can be verified that the wells 04 and 08 have very different compositions from the others.

A possible limitation of this work was the time interval used for data gathering, which was performed in a single year. Collecting data over several years would provide a broader view of water quality and possibly provide other relationships between variables and wells in the multivariate analysis. In this context, it would also be possible to use supervised statistical analysis techniques, which use group discrimination criteria.

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Data availability statement

All data sets were generated or analyzed in the current study.

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References

Baird, R. B.; Eaton, A. D. & Rice, E. W. (Eds.) Standard Methods for the Examination of Water and Wastewater. 23th ed. American Public Health Association, American Water Works Association, Water Environment Federation, Washington. 2017.

Carvalho, F. I. M.; Lemos, V. P.; Dantas Filho, H. A.; Dantas, K. G. F. Avaliação da Qualidade das Águas Subterrâneas de Belém a partir de Parâmetros Físico-Químicos e Níveis de Elementos Traço Usando Análise Multivariada. *Rev. Virtual Quím.* **2015**, *7* (6), 2221–2241. https://doi.org/10.5935/1984-6835.20150132

Celestino, A. E. M.; Cruz, D. A. M.; Sánchez, E. M. O.; Reyes, F. G.; Soto, D. V. Groundwater Quality Assessment: An Improved Approach to K-Means Clustering, Principal Component Analysis and Spatial Analysis: A Case Study. *Water*. **2018**, *10* (4), 437. https://doi.org/10.3390/w10040437

Chaves, H. S.; Morais, D. G.; Dantas Filho, H. A.; Dantas, K. G. F.; Beirao, A. T. M.; Silva, K.P.; Silva, J. N.; Silva, V. F. A.; Silva, P. A.; Carvalho, F. I. M. Aplicação estatística multivariada para a avaliação físico-química na qualidade da água subterrânea na cidade de Parauapebas (Sudeste do Estado do Pará). *Revista Ibero Americana de Ciências Ambientais.* **2020**, *11* (5), 261–272. https://doi.org/10.6008/CBPC2179-6858.2020.005.0025

Charfi, S.; Zouari, K.; Feki, S.; Mami, E. Study of variation in groundwater quality in a coastal aquifer in north-eastern Tunisia using multivariate factor analysis. *Quat. Int.* **2013**, *302*, 199–209. https://doi.org/10.1016/j.quaint.2012.11.002

Ferreira, M. M. C. *Quimiometria*: Conceitos, métodos e aplicações. Editora da Unicamp, 2015. https://doi.org/10.7476/9788526814714

Galvão, M. J. T. G.; Costa Filho, W. D.; Srinivasan, V. S.; Schuster, H. D. M.; Rego, J. C.; Albuquerque, J. P. T. *Comportamento das bacias sedimentares da região semiárida do Nordeste brasileiro. Hidrogeologia da Bacia Sedimentar do Rio do Peixe*. CPRM/UFCG/FINEP, 2005.

Gomes, M. C. R.; Cavalcante, I. N. Aplicação da análise estatística multivariada no estudo da qualidade da água subterrânea. *Águas Subterrâneas.* **2017**, *31* (1), 134–149. https://doi.org/10.14295/ras.v31i1.28617

Harris, D. C. *Análise Química Quantitativa*. LTC, 2017.

Jiang, Y.; Guo, H.; Jia, Y.; Cao, Y.; Hu, C. Principal component analysis and hierarchical cluster analyses of arsenic groundwater geochemistry in the Hetao basin, Inner Mongolia. *Geochemistry*. **2015**, *75* (2), 197–205. https://doi.org/10.1016/j.chemer.2014.12.002

Lyra, W. S.; Silva, E. C.; Araújo, M. C. U; Fragoso, W. D.; Veras, G. Classificação periódica: um exemplo didático para ensinar análise de componentes principais.

Quím. Nova. **2010**, *33* (7), 1594–1597. https://doi.org/10.1590/S0100-40422010000700030

Lopes, T. S. A.; Santos, W. B.; Silva, G. A. B.; Silveira, T. N.; Ferreira, W. B.; Feitosa, P. H. C.; Lima, V. L. A. Effects of the transfer of the São Francisco River waters on the performance of the water treatment plant of Gravatá, Paraíba, Brazil. *Water Supply.* **2022**, *22* (3), 3297–3306. https://doi.org/10.2166/ws.2021.404

Mingoti, S. A. *Análise de dados através de métodos de estatística multivariada*. Editora da UFMG, 2007.

Nnorom, I. C.; Ewezie, U.; Eze S. O. Multivariate statistical approach and water quality assessment of natural springs and other drinking water sources in Southeastern Nigeria. *Heliyon.* **2019**, *5* (1), e01123. https://doi.org/10.1016/j.heliyon.2019.e01123

Pan, C.; Ng, K. T. W.; Richter, A. An integrated multivariate statistical approach for the evaluation of spatial variations in groundwater quality near an unlined landfill. *Environ Sci Pollut Res* **2019**, *26* (6), 5724–5737. https://doi.org/10.1007/s11356-018-3967-x

Rossiter, K. W. L.; Marques, E. A. T.; Oliveira, C. R.; Morais, M. M. Q. M. M. Spatial-temporal evaluation of water quality in Brazilian semiarid reservoirs. *Water Pract. Technol.* **2020**, *15* (1), 92–104. https://doi.org/10.2166/wpt.2020.001

Souza, A. M.; Poppi, R. J. Didactic chemometrics experiment for exploratory analysis of edible vegetable oils by mid-infrared spectroscopy and principal component analysis: a tutorial, part I. *Quím. Nova.* **2012**, *35* (1), 223–229. https://doi.org/10.1590/S0100-40422012000100039

Taşan, M.; Demir, Y.; Taşan, S. Groundwater quality assessment using principal component analysis and hierarchical cluster analysis in Alaçam, Turkey. *Water Supply.* **2022**, *22* (3), 3431–3447. https://doi.org/10.2166/ws.2021.390

Valderrama, L.; Paiva, V. B.; Março, P. H.; Valderrama, P. Proposta experimental didática para o ensino de análise de componentes principais. *Quím. Nova.* **2016**, *39* (2), 245–249. https://doi.org/10.5935/0100-4042.20150166

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Scientific recreations to favor the learning of the periodic table in high school students with incomplete schooling

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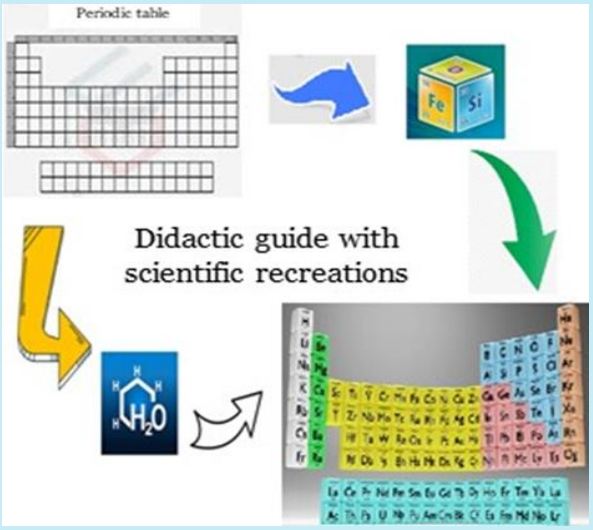
ABSTRACT: Didactic games for science teaching contribute to student learning and break with traditional teaching models. The objective of this study was to implement a didactic guide with scientific recreations to favor the learning of the periodic table in students with incomplete schooling in the 2022–2023 school year. For this purpose, an experimental, field and explanatory research was used. A population study was carried out with 60 students of the first year of high school of the "Velasco Ibarra" Fiscal Educational Unit. The main theoretical and empirical methods were used, as well as descriptive and inferential statistics for data processing, analysis and interpretation. A didactic guide with scientific recreations was elaborated to favor the learning of the periodic table in students with unfinished schooling, which was applied to the students of the "Velasco Ibarra" Fiscal Educational Unit, in the 2022–2023 school year. It was corroborated that the didactic guide with scientific recreations applied significantly improved the students' learning of the periodic table.



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1. Introduction

From the beginning, human beings have been interested in knowing the world around them, trying to explain each of the phenomena existing in nature, which led to what is known today as Chemistry, a branch of the natural sciences, which is present in all aspects of everyday life and, therefore, also in the educational field, although there are certain difficulties in this field, both in teaching and learning.

In this regard, Valdés (2019, p. 15) refers that: "Chemistry is one of the branches of science that brings together a large accumulation of abstract and complex information, which hinders the appreciation and understanding of topics in its teaching, causing deficiency in the development of scientific skills".

Chemistry as a science implies that students who learn by performing a scientific school activity not only recognize new ideas and identify evidence, but also learn to talk and write about it, to give a better meaning to those ideas and experiments (Sanmartí, 2008).

Tang and Rappa (2021) proposed a model intended to support students in the construction of scientific explanations in chemistry, which comprises three main components: (a) the premise: theoretical knowledge that provides the basis for the explanation, (b) the reasoning: logical sequences that follow from the premise, and (c) the result or conclusion: the phenomenon that is explained. According to these authors, since the genre of scientific explanation is not a familiar form of writing for many people, most students find it difficult to write the periodic table in a simple way, as they do not know where to start.

On the other hand, García Posso and Posso García (2017, p. 582) indicate that: "The lack of adequate teacher training has generated behaviorist practices that do not favor student learning, but favor dependence, lack of creativity and inability to think". It is worth mentioning that, under this perspective, Pérez (2018) suggests that, globally, in recent years, in terms of Chemistry teaching, links have been established between structure, properties and practical applications, which generates methodological variations in the teaching-learning process. This shows the need to look for novel methodologies that can really motivate students to learn in a meaningful way.

Therefore, Barahona and Constante (2019), mention that the methodology of the learning and teaching process in the baccalaureate is constituted by the objectives, knowledge, attitudes and values that students must learn, a different way of presenting the contents is sought, using innovative and at the same time everyday resources, with the purpose of achieving true knowledge in students.

The use of games is often considered in the literature as a test of interest when it comes to getting the student to actively participate in teaching and learning. Orlik (2002), in an extensive study on active methodologies in the teaching of science in general, and chemistry in particular, places this resource as one of the most important in this sense.

On the other hand, Yager (1991) points out that "taking part in focused games" places students in a scenario that facilitates their motivation and allows them to work on a wide range of skills. Similarly, didactic games, created individually or in groups, provide students with the opportunity to be creators of their own learning.

In this sense, Mondeja *et al.* (2001) specify a set of qualities and requirements that games meet and make them useful in the development of the teaching and learning process:

1. Games contribute to dynamize the students' activity in many forms of teaching organization, where, once motivated, they develop their cognitive activity;
2. They indirectly improve the efficiency of educational processes, since they demand greater reflective activity on the part of the teacher;
3. They must be used in a planned manner in correspondence with the educational intentions and their implications in the classroom.

Finally, games have two important points in the development of the teaching and learning process, namely: they are a learning tool and, at the same time, a learning strategy, since they mean a different way of working and learning.

According to Torres (2002), didactic games also interest and promote other qualities in students, such as self-control, honesty, security, care and concentration in work, meditation, the search for other ways to win, according to the rules of the game. to play, to initiate, to understand and connect with others.

The different types of games available for chemistry teaching should be explained in different ways. Orlik (2002), for example, distinguishes three major types of games applicable to the classroom, which he calls exercise games, occupational games, and knowledge quiz-type games.

Exercise games can be defined as easy-to-solve minigame problems, usually with pencil and paper, similar in structure to puzzles and word games. As a rule, these games are suitable for individual or small group work. Typical examples are word searches or crossword puzzles (Rannikmiae *et al.*, 1982). The reverse task is

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also feasible, i.e., the student himself is the one who designs new crossword puzzles with chemistry or science terms and concepts.

Occupational games consist of giving each student a *job*, which they must successfully defend and explain to their peers. For example, occupational games have been designed based on professions in the chemical industry around the production of organic compounds ammonia sulfuric acid, etc. A variant is the class-consultation, where only three roles are assigned to the students: teacher, assistant and inspector, who must answer questions posed by the rest of the class on a particular topic. This variant allows for better preparation of the group before an exam. A third option is to organize the occupational game in the form of a theater, which increases the motivation of the students.

The third and last type of games are quizzes that can be organized both in chemistry classes and in an extracurricular context (Franco-Mariscal *et al.*, 2012). In general, this type of game resembles a television program in many countries and may involve two or more teams of students. The game is preceded by a preparatory stage in which the teacher formulates a task to research both the chemical and general scientific literature on the topic. Depending on your level (high school or college) the questions should be of different difficulty.

Regarding the teaching of the Periodic Table, a traditional, theoretical and memoristic way has been generalized, which causes disinterest in students to learn and understand Chiriboga (2022). In this way, it can be said that, the activities of a teacher in the classroom can be difficult, since it requires planning, an organization with a favorable environment that allows teaching and learning according to the reality of each educational institution and therefore the students. Classroom management involves several factors to develop properly helping to improve student learning.

In Ecuador, there are many shortcomings in the educational context, not having found a global project that meets all the needs of the educational community. In view of this, Rengifo Ávila and Espinoza Freire (2019, p. 177) state:

> Ignorance of the importance of education for the development of the country leads to prioritize other sectors, mitigating the formation of citizenship. / The above brings us closer to a painful reality in which there are countless problems at the level of education in Ecuador, but it is complex to understand why they are not being solved, if they are key pieces of the country's development.

Another problem in Ecuador is student dropout, which is also caused by different factors: economic, labor, social and personal. In Ecuador, there are 5.7 million people who are in a situation of illiteracy or unfinished schooling, among which we have 692 316 people who require literacy, 979 743 people who require post-literacy, 3 132 586 people who require higher basic education and 927 468 who require Baccalaureate (Ministry of Education, 2019).

The Ministry of Education, as the institution in charge of guaranteeing the right to education, serves the population with incomplete schooling and educational backwardness through extraordinary educational services in three modalities: face-to-face, blended and distance.

In view of the above, the General Regulations to the Organic Law of Intercultural Education of Ecuador (Ministry of Education, 2015) in Article 151 states that:

> The evening session, which can only be offered to persons fifteen years of age or older, applies a blended learning modality through which a special curriculum is developed that determines 70% for face-to-face academic activities and 30% for academic activities of independent work under teacher supervision... (p. 46).

In another aspect, in evening education, when presenting students over the age of 18 with multiple daily responsibilities, it is difficult to capture their attention, so it is necessary to implement teaching methodologies different from the usual ones. In this regard, Rodríguez Lorbada (2017) states that there are different theories for adult learning, including: andragogy, transformational learning and experiential learning, and each of these theories converge in the same purpose: to develop learning techniques and experiences that are effective for adult learners.

It is imperative to change traditional methodologies for others that involve the students as the main actors in their own teaching-learning process, with the support of the teacher as mediator and strategist in the application of playful activities that reinforce learning (Galagovsky, 2007).

On the other hand, in the province of Manabí, specifically in the canton of Portoviejo, there are predominantly families of middle and low social strata that have educational lags, who, despite the inconveniences that have been presented to these people, decide to continue their studies and are called students with unfinished schooling, for which there are night educational institutions that ensure studies in an

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extraordinary way, adjusting the curricular content with the prioritization established by the Ministry of Education to serve this student population. One of these institutions is the "Velasco Ibarra" Fiscal Educational Unit.

Within the institutional reality of the "Velasco Ibarra" Fiscal Educational Unit, there are different problems, as follows:

- Few scientific-recreational activities in theoretical subjects;
- Insufficient learning skills in students;
- Scarce pedagogical resources for the correct teaching of the different subjects;
- Low student interest in classroom activities.

In this institution there are multiple insufficiencies in the teaching and learning of the periodic table. In virtue of the above, the objective of this research is to implement a didactic guide with scientific recreations to favor the learning of the periodic table in students with unfinished schooling in the first year of high school at the "Velasco Ibarra" Fiscal Educational Unit.

2. Methodology

The research was conducted using a mixed (qualitative-quantitative), explanatory approach and an experimental design. The main theoretical methods were used, namely: historical-logical, analysis-synthesis, inductive-deductive and hypothetical-deductive, to understand the object of study in its development, its history and logic, to discover the essential relationships and general characteristics among them, to determine generalizations and empirical laws, and to reach new conclusions and empirical predictions.

The following empirical methods and techniques were used to collect data on the indicators defined by each relevant variable: scientific, participant and covert observation, questionnaire, semi-standardized interview, measurement and the social experiment, due to the largely subjective nature of the object of study and the field of research, and the influence of multiple factors that are difficult to control.

For the processing, analysis and interpretation of the data collected, descriptive statistics were used, through the calculation of percentage values, measures of central tendency, measures of dispersion and construction of graphs. A population-based study was carried out, since 100% of the students of the First Year of the Unified General High School of the "Velasco Ibarra" Fiscal Educational Unit participated in the research, amounting to 60 students.

A quasi-experimental design was used, since a control group and an experimental group were configured. The research was developed in three stages: i) a pretest was made to the students of the two groups (control and experimental) to diagnose the knowledge and previous learning about the chemical elements of the periodic table; ii) the teaching and learning process was developed to the control group with the traditional method and to the experimental group the proposed strategy was applied with the resources and applications considered about the chemical elements of the periodic table and; iii) a post-test was applied to check the feasibility and relevance of the implemented strategy.

A didactic guide based on scientific recreations was elaborated to favor the learning of the periodic table in high school students with incomplete schooling, in a collaborative and team way, which consisted of six games, namely: Periodic table quiz, Chemistry App, Quimitris, Puzzle, Periodic table bingo and the atomic deck, all of them simple games, to experience a higher level of motivation and satisfaction with participative learning.

The research variables were: scientific recreations (independent variable) and learning the periodic table (dependent variable). Their operationalization appears in Table 1.

Table 1. Operationalization of relevant variables of the research.

Variable	Dimensions	Indicators	Techniques and instruments
Independent variable Playful activities	Attitudinal	Level of preparation on the use of technological resources in their learning	Survey
	Motivational	Students' level of motivation	Survey
	Aptitude	Acceptance of the ludic resources for their learning	Survey
Dependent variable Learning the periodic table	Academic performance	Percentage of students passed Average grade point average	Pretest Posttest

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The extraneous or extraneous variables identified were: i) teachers' motivation towards the changes, ii) students' motivation, iii) students' previous knowledge about the games and, iv) students' previous knowledge. The following actions were taken to control these variables:

- According to the motivation of teachers, work was done in two directions: a) teachers were motivated to use games for learning the periodic table, and b) teachers were prepared to motivate students about the importance and possibility of learning through games, for which workshops were held on the importance of this and the potential of playful activities to promote learning;
- The motivation of the students was controlled through practical activities, individually and in groups, about the relevance and usefulness of learning chemistry through playful activities, which included several examples of how to learn through didactic games. In this way, the students showed greater interest and paid more attention in the demonstrative classes conducted;
- With respect to the students' prior knowledge about the games, in the same practical activities executed to improve their motivation, several of them were demonstrated with some of the same games they would use during the teaching-learning process of the periodic table;
- Regarding the students' previous knowledge, an initial diagnosis was made and, based on the results of the same, several academic activities were carried out to level the students in those learning skills they should already have to start learning the contents taught in the subject of the periodic table.

3. Results and discussion

Based on the theoretical and methodological foundations and the contributions of the authors, this didactic guide with scientific recreations was elaborated to favor the learning of the periodic table in students with incomplete schooling in the first year of high school, as shown in Table 2.

Table 2. Didactic guide with scientific recreations to favor the learning of the periodic table in students.

Game	Description
Periodic table quiz	For teaching the elements of the periodic table in an interactive and simple way. It offers six types of game: guess the number of the element, its name or the group number to which they belong. All accompanied by a system of achievements and levels. It is free and compatible with Android devices.
Chemistry App	It has all the information about the elements of the periodic table. By touching any element, you can access its relevant data, allowing you to acquire knowledge and complete information in a simple way. It also contains additional tools to solve chemical reactions.
Quimitris	It is a game based on the classic Tetris for learning the elements of the periodic table in a fun way. The tiles, consisting of one, two, three or four chemical elements, fall from the top of the board and must be placed correctly on the periodic table. The game is divided into different levels that progressively increase in difficulty.
Puzzle	It consists of making a periodic table in three dimensions like a puzzle, where each square is a cube and, on each side, different characteristics of each element are represented: 1) name, 2) symbol, 3) atomic number, 4) photograph of the element, 5) representation of food, materials and medicines in whose composition the element is found, 6) group and period.
Periodic table bingo	Called Quica, it is a game of chance that consists of putting into a bag or drum, a certain number of chips, which contain the atomic number and symbol of a specific chemical element. The game is individual, so each student will have a cardboard, which has the symbol and atomic number of a chemical element at random.
The atomic deck	The atomic deck is a set of cards, arranged by color, with information about a chemical element, such as: symbol, atomic number, period, group, oxidation states, uses and applications. Students will have three cards and must form a word with the symbol of the chemical elements present on them.

The results of the survey applied to the students on the use of didactic tools using technologies and the realization of ludic activities to favor learning, corroborated that most of the Chemistry teachers do not use auditory didactic resources in their classes to reinforce the content on the chemical elements of the periodic table, knowing that these resources help to improve student learning, since of the total number of respondents, 53% affirm that the teachers do not use auditory didactic resources in the class and another 35% refer that they almost never or sometimes use them. Only 12% stated that they almost always use these resources (Table 3).

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Table 3. Absolute (A.F.) and relative frequency (R.F.) of responses to survey questions.

No	Questions	Always		Almost always		Almost always Sometimes		Almost never		Never	
		A.F.	R.F.	A.F.	R.F.	A.F.	R.F.	A.F.	R.F.	A.F.	R.F.
1	How often are auditory materials such as CDs and recordings used in Chemistry class?	0	0	7	12%	16	27%	5	8%	32	53%
2	Are slides, images, graphic organizers, etc., projected for the explanation of the elements of the periodic table?	10	17%	7	11%	10	17%	9	15%	24	40%
3	In chemistry class, do you practice the chemical elements of the periodic table using three-dimensional materials such as puzzles or 3D cubes?	1	2%	10	17%	14	23%	9	15%	26	43%
4	Do you find it useful to learn about the chemical elements of the periodic table through games?	19	32%	12	20%	17	28%	9	15%	3	5%
5	Are the lectures given by your chemistry teacher understandable at any time?	4	7%	5	8%	29	48%	21	35%	1	2%

In this sense, Blandín and Solórzano (2018) emphasize the incorporation of innovative strategies in the teaching-learning process of the chemical elements of the periodic table, because for the students this subject is very memoristic, with little understandable data, so it causes fear of the unknown, because of the little or little transmission of what was learned with the everyday, especially because of its complexity, which lies in that concepts with non-visual characters such as the atom must be explained.

Fifty-five percent of the respondents never and almost never the teachers project slides, images, graphic organizers and others, for the explanation of the elements of the periodic table; and only 28% of the students refer that they always or almost always do it. This corroborates that most teachers do not use, or do it very little, information technologies in the teaching-learning process of this subject, probably because this subject is usually complicated by the amount of information it has and the relationship that exists between it (Barazarte and Jerez, 2020).

Fifty-eight percent of the students stated that their teachers have never or almost never implemented three-dimensional materials such as puzzles or 3D cubes in their classes on the periodic table, while only 19% always or almost always do so, despite the fact that 52% of the students stated that they always or almost always find it useful to learn through games and that only 15% of the students stated that they understand the teacher. This shows that most teachers do not use, or do it very little, playful activities (games) to teach the theory and practice of the periodic table, despite the potential that these have to promote meaningful learning of students, in contrast to what was stated by Barazarte and Jerez (2020), who point out that teachers should use more creativity in this subject with entertaining and challenging activities for students, in order to facilitate their learning.

Some measures of central tendency and dispersion of the results of the pretest and posttest student scores, after applying the proposal to the experimental group and developing the process in the traditional way with the control group, are shown in Table 4.

Table 4. Descriptive statistics of the results of the pretest and posttest to the students.

Groups	Evaluation	Range	Minimum	Maximum	Median	Mean	σ
Control group	Pretest	6.00	1.00	7.00	4.00	4.00	1.4881
	Posttest	5.00	2.00	7.00	5.00	4.83	1.1805
Experimental group	Pretest	5.00	1.00	6.00	4.00	3.87	1.2313
	Posttest	4.00	5.00	9.00	8.00	8.10	0.9076

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In the control group, both in the pretest and posttest, as well as in the pretest of the experimental group, the great majority of the grades obtained by the students were at the low level (< 7.00 points). However, once the didactic strategy was applied, of the experimental group, 80.6% of the student's achieved grades of the high level (≥ 8.00 points); therefore, only six students of the group obtained grades of the medium level in the posttest.

In the pretest, in both groups, similar mean values were obtained. The analysis of the averages obtained by the students in the grades of both groups in the pretest, corroborate that they had a similar preparation in terms of previous knowledge, with which they started the teaching-learning process of the studied subject, so this previous learning did not influence the final results. This statement was confirmed by means of the Student's t-test for related samples, which reported a p value = 0.842 ($p > 0.05$); therefore, it can be affirmed with 95% confidence that there are no statistically significant differences between the means obtained by the students in the pretest in the control and experimental groups.

On the other hand, from the analysis of the means obtained by the students in the grades of both groups in the posttest, it was found that when applying a Student's t-test for related samples, a value of $p < 0.05$ was obtained; so it can be affirmed with 95% confidence that there are statistically significant differences between the means obtained by the students in the posttest in the control and experimental groups, which corroborates that the recreations applied did improve the academic performance of the students in terms of the periodic table. This agrees with Arce Urbina (2022), who points out that experimentation has great value in the teaching of natural sciences, since it is essential for students to assimilate a subject, exposing them to different and novel experiences so that they achieve greater motivation in their learning.

Likewise, from the analysis of the means obtained by the students in the pretest and posttest grades of the control group, it was found that when applying a Student's t-test for related samples, a value of $p = 0.268$ ($p > 0.05$) was obtained; so that it can be affirmed with 95% confidence that there are no statistically significant differences between the means obtained by the students in the pretest and posttest in the control group, which corroborates that the students of the control group did not significantly improve their academic performance in learning the periodic table.

This result corroborates Cuichán (2018), who refers that, in order to improve student learning in the subject of Chemistry, it is necessary that teachers plan their classes with strategies that allow students to assimilate it, in a more attractive, interesting and participatory way during the teaching-learning process, in order to achieve meaningful learning. In this sense, Orlik (2002) refers those teachers should incorporate into the curriculum, didactic and playful strategies that allow students to acquire knowledge and skills that are more attractive, interesting and participatory during the teaching-learning process, in order to achieve meaningful learning.

4. Conclusions

The elaboration of a didactic guide with scientific recreations to favor the learning of the periodic table in students is an effective tool, since it is based on simple games that help students to better understand the concepts on this topic and apply them in practical situations, experience a higher level of motivation and satisfaction with learning, work collaboratively and as a team, to benefit their participation and exchange of knowledge among them.

The implementation of the didactic guide with scientific recreations to favor the learning of the periodic table in high school students with incomplete schooling, improved the academic performance and the motivation and attitude of the students towards their learning, as well as their perception and satisfaction with respect to the usefulness of the games to favor learning.

Authors' contribution

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Data availability statement

The data will be available upon request.

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References

Arce Urbina, M. E. The Value of Experimentation in the Teaching of Natural Sciences. The Science Workshop for Children at the Atlantic Campus of the University of Costa Rica: An Experience to Share. *Education Journal.* **2019**, *26* (1), 147–154.

Barahona, A.; Constante, E. Methodological strategies in the Teaching-Learning Process of the subject of Chemistry, unit 2, in the International Baccalaureate Diploma Program, Eloy Alfaro Educational Unit, period 2018-2019. Degree thesis, Central University of Ecuador, **2019**.

Barazarte, C.; Jerez, E. Application of the periodic bingo game as a strategy for the teaching-learning of the periodic table in the third year of high school. Degree thesis, University of the Andes, **2020**.

Blandín, F.; Solórzano, R. Relevance of innovative strategies in the teaching-learning process of the chemical elements of the periodic table. Degree thesis, Central University of Venezuela, **2018**.

Chiriboga, N. Management of digital strategies in the teaching-learning of the Periodic Table of Chemistry, First Year of General Unified High School, of the Municipal School "Juan Wisneth", DM of Quito, 2021-2022. Degree thesis, Central University of Ecuador, **2022**.

Cuichán, S. Didactic strategies for the significant learning of block number 2 of chemistry in first year students of unified general high school of the Colegio Fisco Misional "San Jerónimo" of Píntag in the school year 2013-2014. Degree thesis, Central University of Ecuador, **2018**.

Franco-Mariscal, A. J.; Oliva-Martínez, J. M.; Bernal-Márquez, S. A literature review on the role of educational games in the study of the chemical elements.: Part I: Games for knowledge of the Periodic Table. Educ. Quím. **2012**, *23* (3), 338–345.

Galagovsky, R. Teaching Chemistry vs. Learning Chemistry. An equation that is not balanced. *Living Chemistry*. **2007**, *6* (Sup), 1–13.

García Posso, B. E.; Posso García, L. M. Didactic situations in the teaching of chemical bonding. *Educere.* **2017**, *21* (70), 581–592.

Ministry of Education. *General Regulations to the Organic Law of Intercultural Education of Ecuador*; Ministry of Education, **2015**.

Ministry of Education. *Education for Youth and Adults*; Ministry of Education, **2019**.

Mondeja, D.; Zumalacárregui, B.; Martín, M.; Ferrer, C. Didactic games: useful in higher education? *University Pedagogy*. **2001**, *6* (3), 65–76.

Orlik, Y. *Chemistry:* active teaching and learning methods; Editorial Iberoamérica, **2002**.

Pérez, R. A different way of teaching inorganic chemistry. *Cuban J. Chem.* **2018**, *27* (2), 197–203.

Rannikmiae, M.; Tildsepp, A.; Sushko, A. *Elements of didactic games in chemistry classes*; Chemistry and School, **1982**.

Rengifo Ávila, G. K.; Espinoza Freire, E. E. Study on problems in Ecuadorian education and educational policies, 1990-2018. *Metropolitan J Appl Sci.* **2019**, *2* (3), 175–182.

Rodríguez Lorbada, G. Adult learning theories to design effectively. Guillermo Rodríguez Lorbada, **2017**. https://lorbada.com/blog/2017/04/22/teorias-de-aprendizaje-para-adultos-para-disenar-con-eficacia (accessed 2022-02-16).

Sanmartí, N. Writing to learn science. *Aula de Innovación Educativa*. **2008**, *175*, 29–32.

Torres, C. M. The game: an important strategy. *Educere*. **2002**, *6* (19), 289–296.

Eclética Química, vol. 48, n. 4, 2023, 48-56
ISSN: 1678-4618
DOI: 10.26850/1678-4618eqj.v48.4.2023.p48-56

Tang, K.-S.; Rappa, N. A. The role of metalanguage in an explicit literacy instruction on scientific explanation. *Int. J. Sci. Math. Educ.* **2001**, *19* (7), 1311–1331. https://doi.org/10.1007/s10763-020-10121-6

Valdés, G. *Application of augmented reality for the elaboration of chemistry experiments as a support tool in the teaching of their reactions*; University of Cundinamarca, **2019**.

Yager, R. E. The constructivist learning model: Towards real reform in science education. *The Science Teacher.* **1991**, *58* (6), 52–57.

Eclética Química, vol. 48, n. 4, 2023, 48-56
ISSN: 1678-4618
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