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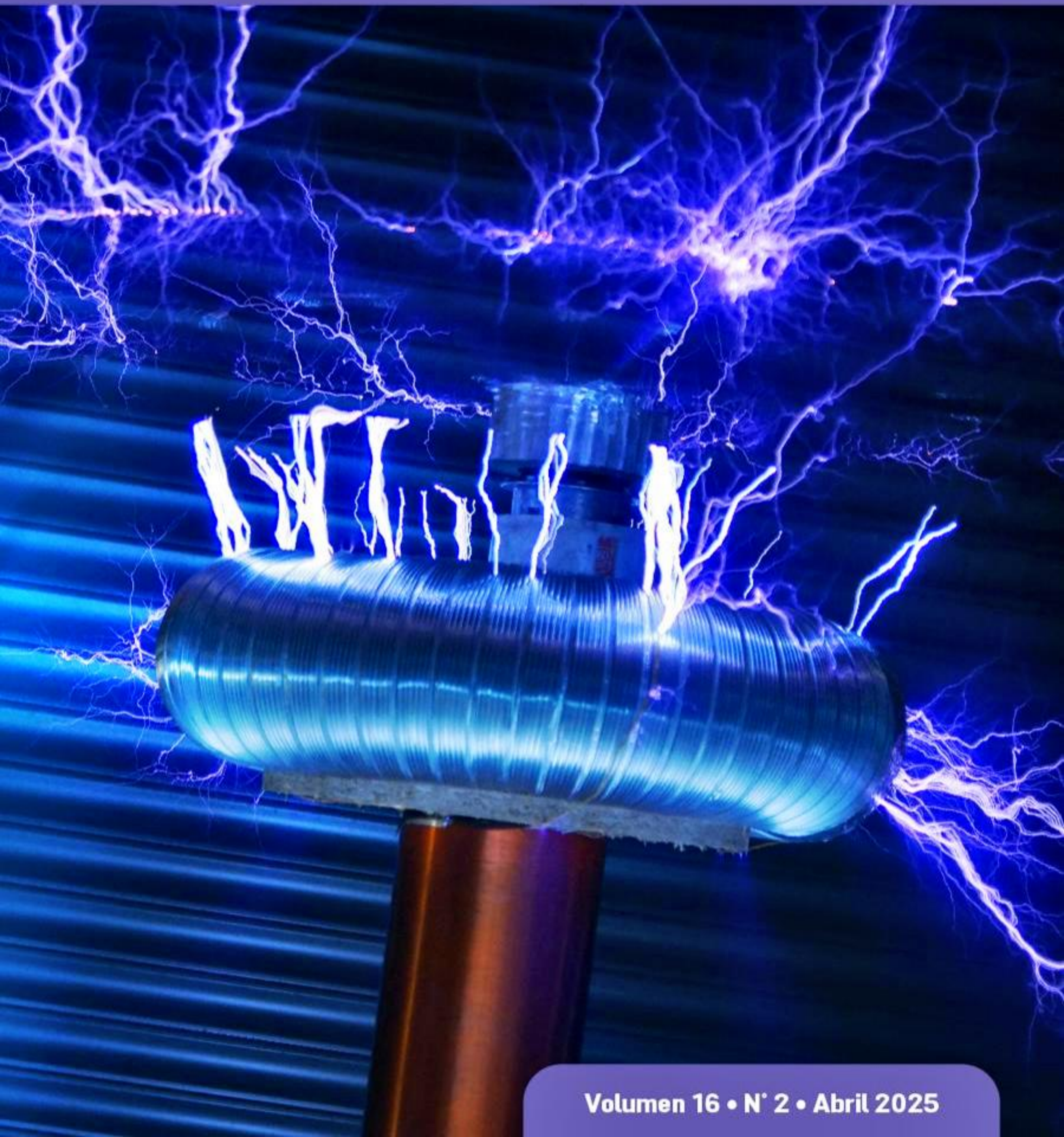

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Editorial

It is a pleasure to present Volume 16, Issue 2 of the Enfoque UTE journal, which features a selection of six high-quality research articles. All contributions included in this edition have undergone a rigorous peer review process by at least 2 national and international experts.

In this issue, we are pleased to highlight the study by Fabian Diaz et al., which presents a novel approach to fault detection in axial piston hydraulic pumps by integrating principal component analysis and silhouette analysis with clustering algorithms.

Another important contribution is the work of Kevin Guanoluisa et al., who explores the development and evaluation of a biofertilizer based on the Anabaena-Azolla complex. This study focuses on sustainable agriculture and presents significant findings on growth performance and nitrogen concentration of biofertilizer.

Furthermore, in the industrial field, Tomás Marín, presents a bibliometric analysis on the use of artificial neural networks in the oil and gas industry from 2020 to 2024. His research provides a comprehensive overview of scientific production, highlighting trends in applications such as exploration, drilling, production, and emissions control.

Likewise, this issue presents the study of Andres Perez-Gonzalez et al., which investigates the removal of a mixture of emerging pharmaceutical contaminants assisted by a fixed TiO2 support in a photocatalytic process. This study contributes to the growing field of environmental remediation and water treatment.

Jorge García et al. present a study on human resources as a critical success factor for quality and sustainability in the industry. His research underscores the importance of workforce management in achieving long-term industrial sustainability.

Finally, Fernando Toapanta-Ramos contributes with a numerical study using computational fluid dynamics (CFD) on heat sinks for electronic components. His research provides insights into thermal management solutions to improve the efficiency of electronic devices.

We invite readers to explore these six contributions, each of which reflects the dedication of their respective authors to advancing scientific knowledge across a diverse range of fields. These studies not only deepen our understanding of key topics, but also offer practical solutions to pressing global challenges.

Dr. Oscar Martínez Mozos
Universidad Politécnica de Madrid
Editor-in-Chief

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Editorial

Es un placer presentar el Volumen 16, Número 2 de la revista Enfoque UTE, el cual incluye una selección de seis artículos de investigación de alta calidad. Todas las contribuciones incluidas en esta edición han sido sometidas a un riguroso proceso de revisión por pares realizado por al menos dos expertos nacionales e internacionales.

En esta edición nos complace destacar el estudio de Fabian Diaz et al., que presenta un enfoque novedoso para la detección de fallas en bombas hidráulicas de pistones axiales mediante la integración del análisis de componentes principales y el análisis de silueta con algoritmos de agrupamiento.

Otra contribución importante es el trabajo de Kevin Guanoluisa et al., que explora el desarrollo y la evaluación de un biofertilizante basado en el complejo Anabaena-Azolla. Este estudio se centra en la agricultura sostenible y presenta hallazgos significativos sobre el rendimiento del crecimiento y la concentración de nitrógeno en el biofertilizante.

Además, en el ámbito industrial, Tomás Marín presenta un análisis bibliométrico sobre el uso de redes neuronales artificiales en la industria del petróleo y gas entre 2020 y 2024. Su investigación proporciona una visión integral de la producción científica, destacando tendencias en aplicaciones como la exploración, perforación, producción y control de emisiones.

Asimismo, en este número se presenta el estudio de Andrés Pérez-González et al., que investiga la eliminación de una mezcla de contaminantes farmacéuticos emergentes mediante un soporte fijo de TiO2 en un proceso fotocatalítico. Este estudio contribuye al creciente campo de la remediación ambiental y el tratamiento de aguas.

Jorge García et al. presentan un estudio sobre los recursos humanos como un factor crítico de éxito para la calidad y sostenibilidad en la industria. Su investigación resalta la importancia de la gestión del talento humano en la consecución de la sostenibilidad industrial a largo plazo.

Finalmente, Fernando Toapanta-Ramos aporta un estudio numérico utilizando dinámica de fluidos computacional (CFD) sobre disipadores de calor para componentes electrónicos. Su investigación proporciona información sobre soluciones de gestión térmica para mejorar la eficiencia de los dispositivos electrónicos.

Invitamos a los lectores a explorar estas seis contribuciones, cada una de las cuales refleja la dedicación de sus respectivos autores en el avance del conocimiento científico en diversas áreas. Estos estudios no solo profundizan nuestra comprensión de temas clave, sino que también ofrecen soluciones prácticas a desafíos globales urgentes.

Dr. Oscar Martínez Mozos
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Fault detection in axial piston hydraulic pumps: integrating principal component analysis with silhouette-based cluster evaluation

Fabian H. Diaz Palencia[1], Carlos Borrás[2], Cecilia E. García Cena[3]

Abstract **—This paper presents an approach integrating principal component and silhouette analysis with clustering algorithms for fault detection in hydraulic systems. The methodology was validated through a study in which vibration and pressure signals were collected under normal and fault conditions. These signals were then processed through filtering and normalization, followed by dimensionality reduction using principal component analysis. The resulting lower-dimensional feature vectors retained the critical characteristics of both normal and faulty conditions and were subsequently fed into a clustering algorithm. The quality of the resulting clusters was evaluated using silhouette analysis, which offers a reliable means of assessing cluster quality and visualising the outcomes of fault classification. The study demonstrates the effectiveness of this method in accurately representing the patterns of normal and malfunctioning hydraulic pump conditions, ultimately leading to successful diagnostic results.**

Keywords: **Principal Component Analysis; Silhouette Analysis; Failure Detection; hydraulic piston pump.**

Resumen **— Este artículo presenta un enfoque que integra el análisis de componentes principales y el análisis de siluetas con algoritmos de agrupamiento para la detección de fallos en sistemas hidráulicos. La metodología se validó a través de un estudio en el que se recopilaron señales de vibración y presión en condiciones normales y de fallo. Estas señales fueron procesadas mediante filtrado y normalización, seguidos de una reducción de la dimensionalidad con el análisis de componentes principales. Los vectores de características de menor dimensión resultantes conservaron las características críticas tanto de las condiciones normales como de las defectuosas y posteriormente se introdujeron en un algoritmo de agrupación. La calidad de los conglomerados resultantes se evaluó con el análisis de siluetas, que ofrece un método fiable para evaluar la calidad de los conglomerados y visualizar los resultados de la clasificación de fallos. El estudio demuestra la eficacia de este método a la hora de representar con precisión los patrones de las condiciones normales y defectuosas de las bombas hidráulicas, lo que en última instancia conduce a resultados de diagnóstico satisfactorios.**

Palabras clave: **Análisis de Componentes Principales; Análisis de Silueta; Detección de fallas; Bomba Hidráulica de Pistones.**

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I. INTRODUCTION

FAULT monitoring and diagnosis in dynamic systems is a key challenge in industrial engineering, particularly in the analysis of sensor data. The axial piston hydraulic pump is a critical component within hydrostatic systems [1]; it is used as equipment to transmit power in various applications, and its good performance depends on the success and efficiency of the operations in which it is involved within industrial processes. For this reason, companies invest significant efforts and capital in maintenance issues to take advantage of or prolong to the maximum its operation; early detection of failures in the components that integrate it has been a constant research task in recent years. This task consists of determining the type of failure, and for this purpose, it is possible to distinguish three main approaches [2] [3] [4].

- Diagnostic systems for hydraulic systems based on the developed model of the diagnosed system.
- Diagnostic systems for hydraulic systems based on signal analysis.
- Diagnostic systems for hydraulic systems based on knowledge or so-called intelligent fault identification.

Fault detection using knowledge-based methods is a heuristic process. System characteristic values are used to extract features under normal and erratic conditions; once the features are extracted under both conditions, they are compared and the change detection methods are applied. Artificial neural networks, fuzzy logic, principal component analysis and neuro-fuzzy methods can be considered knowledge-based [5]. This paper focuses on applying Principal Component Analysis (PCA) for anomaly and fault detection in time series data, followed by a detailed analysis using t^2. In addition, silhouette plot analysis is included to assess the quality of the clusters generated from the PCA scores. The aim is to provide a robust methodology for detecting system failures from vibration data or other sensor measurements.

II. BACKGROUND

Several methods have been employed for fault detection and diagnosis in hydraulic systems. Table I compares various techniques used for this purpose. Each process is described in terms of its basic functionality, specific applications in the context of hydraulic systems, key advantages, and inherent limitations. On the opposing side., Table II shows some techniques for detection or diagnosis. of faults in hydraulic systems based on the methods previously described.

A. Principal Components Analysis as a Methodology for Fault Detection

The Principal Components Analysis (PCA) method, introduced by Pearson in 1901 and Hoteling in 1933, is a statistical tool designed to reduce the dimensionality of a dataset containing multiple interrelated variables while preserving as much variation as possible. This is achieved by transforming the original variables into a new set of uncorrelated variables known as principal components. These components are ordered, with the first retaining most of the variation present in the original variables [6].

PCA has proven to be a powerful tool for detecting faults in complex systems, especially in industrial processes and machinery. PCA is well-suited for identifying anomalies in high-dimensional datasets. By projecting new data onto the lower-dimensional space defined by the principal components, deviations from normal operation patterns can be readily identified. This approach allows for the timely detection of subtle changes in system behavior that may indicate the onset of faults. The ability of PCA to handle large datasets, reduce noise, and provide interpretable results has led to its increasing popularity for fault detection (see Fig. 1) across various industries, including manufacturing, chemical processing, and mechanical systems.

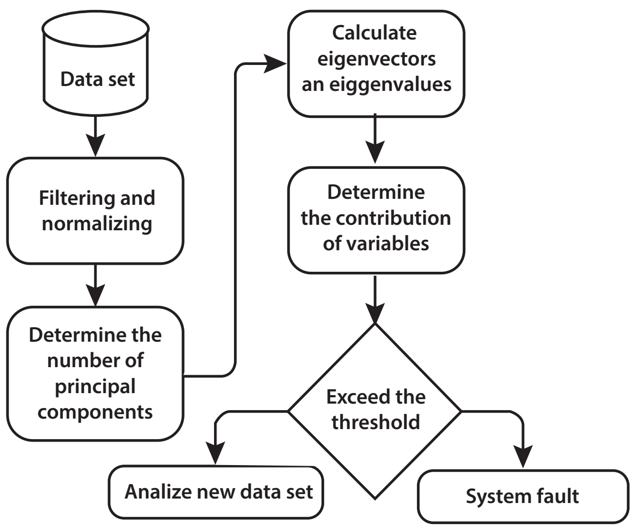

Fig. 1. Typical diagnostic methodology by PCA.

The article [7] mentions that PCA applications in multivariate process failure diagnosis started in the 1990s, and to date, it is still implemented in conjunction with other techniques or methodologies. The idea is to use sensor data and/or variables that describe the operation of devices, processes, or systems and apply PCA to identify the main components that explain the most significant amount of variability in the data to identify patterns or relationships that may indicate the presence of a fault or erratic operation.

L. Siyuan et al., in [8] show a study on the application of PCA for fault detection in Hydraulic Pumps, and in [9] combines Rough Set (RS) and PCA to diagnose faults based on the energy characteristics of Vibration signals also in hydraulic pumps.

M. Atoui et al., in [10] apply Bayesian Networks (BN) and PCA, BN and 4381 T^2-SPE for fault detection, validating both methodologies using the Tennessee Eastman Process, showing that both methods produce the same performance at the time of fault detection.

Villegas et al. in [11] describe the PCA application for fault detection and diagnosis in a real plant. The approach includes a PCA model for each system behavior, i.e., models under normal and fault conditions. It demonstrates that detecting and identifying level sensor failures and clogging in a two-communicating tank system is possible. The paper [29] presents a multimode process monitoring technique that integrates density peak clustering and kernel principal component analysis with a multi-strategy zebra optimization algorithm. The proposed method enhances mode identification accuracy and fault detection capabilities in dynamic industrial processes. Experimental validation demonstrates the method's superiority over traditional techniques, achieving high fault detection rates and low false alarm rates across various scenarios, particularly in identifying transition modes.

The study presented in [12] introduces an innovative approach for diagnosing faults in grid-connected photovoltaic systems by combining feature extraction techniques like the Salp Swarm Algorithm with supervised machine learning classifiers. The model's performance is compared against traditional methods such as PCA and Kernel PCA. The findings demonstrate that the model achieves a diagnostic accuracy of over 99 % and greatly enhances computational efficiency compared to PCA and KPCA. This improvement is particularly notable for fault classification in nonlinear systems where PCA and KPCA are less effective.

The research detailed in [13] is centered on creating a fault diagnosis and location system for nuclear plant equipment. It utilizes PCA to reduce the dimensionality of sensor data from 70 to 21 dimensions, resulting in improved classification accuracy during the training of a Residual Network, with a peak accuracy of 98.59 %. In a study referenced as [20], Diaz used PCA for detecting failures related to loss of volumetric efficiency and applied SVM to classify the severity of failure in an axial piston pump. The study yielded results close to 99 %.

Zhao et al. [14] propose a new fault diagnosis method based on PCA. First, they transform the vibration signal to the frequency domain. Then, they use the PCA method to reduce the dimension of the feature matrix. Finally, the reduced feature vector is fed into another model to diagnose faults in a rotating machinery bench.

Cárdenas et al. [15] developed a PCA-based approach to detect and categorize faults in a natural gas engine. Their algorithm analyzed alarm bursts to distinguish normal system behavior from failures. The results they obtained were quite promising and outperformed the existing methods used by operators.

TABLE I
METHODOLOGIES FOR FAULT DETECTION

Methodology	Description	Application in Hydraulic Systems	Advantages	Limitations
Support Vector Machines	Classification technique that finds the best margin of separation between classes in a high-dimensional space.	Classification of system status as “normal” or “anomalous” based on sensor data characteristics.	Effective in handling non-linear data; high classification accuracy.	May be sensitive to kernel choice; may not scale well with large data sets.
Artificial Neural Networks	Computational models inspired by the human brain consist of layers of nodes (neurons).	Modeling complex and nonlinear relationships between variables to predict failures based on historical data.	Ability to learn complex relationships; adaptability to different types of data.	Require large amounts of data for training; risk of overfitting.
Convolutional Neural Networks	Deep neural networks are designed to process structured data in the form of images.	Analysis of sensor data or thermal image patterns to identify features that indicate faults.	Efficient in feature extraction; suitable for high-dimensional data.	They require high computational power and training time; they require labeled data.
Recurrent Neural Networks	Networks are designed to handle sequential data and capture temporal dependencies.	Time series analysis of sensor data to detect failure patterns over time.	Capture temporal dependencies; effective for sequential data.	Complexity in training; risk of long-duration gradients and fading.
Decision Trees and Random Forests	Prediction models that divide data into nodes based on binary questions combine multiple trees.	Classification and prediction of failures, combining the output of several trees for more robust decisions.	Easy to interpret; good accuracy; reduce the risk of overfitting.	They can be prone to overfitting without proper adjustment; they may require a lot of training time.
Clustering Algorithms	Group data based on similarities and patterns.	Identification of patterns and anomalies in sensor data that may indicate faults.	No predefined labels are required; suitable for detecting unknown patterns	Sensitive to the number of clusters; may not handle noisy data well.
Principal Component Analysis	Dimensionality reduction technique that transforms data to a new space.	Reduced data complexity to improve the efficiency of other fault detection algorithms.	Simplifies complex data; facilitates visualization of patterns.	May lose relevant information; not always suitable for non-linear data.
Model-Based Methods	They use mathematical models of the system to predict expected behavior and detect anomalies.	Comparison of actual data with the mathematical model to detect deviations that indicate failures.	Accuracy in anomaly detection based on a detailed understanding of the system.	It requires accurate and detailed models, but it can be complex to implement.
Expert and Rule-Based Systems	They use predefined rules and expert knowledge to make decisions and diagnose failures.	Fault diagnosis is achieved by applying specific rules and heuristics that reflect expert knowledge.	Apply domain-specific knowledge; easy to interpret.	Limited by predefined knowledge; cannot adapt to new situations easily.
Anomaly Detection Methods	They focus on identifying significant deviations from normal system behavior.	Using statistical and machine learning techniques, identifying anomalous behaviors that could indicate failures.	Effective in detecting unexpected behavior; can be adapted to different data types.	May generate false positives; require good definition of what constitutes an anomaly.

TABLE II
FAULT DETECTION METHODS AND THEIR CONTRIBUTIONS IN HYDRAULIC SYSTEMS

Article	Fault Type	Analysis Method	Problems Encountered	Contribution
[16]	Fault in the control valve, displacement regulation mechanism, and rotating group.	Kalman Filter with Unknown Input and Residual Evaluation Based on cumulative sum.	Complexity in estimating the swashplate moment and sensitivity to operating conditions.	Improves fault detection sensitivity and speed by considering uncertainties in the swashplate.
[17]	Wear of the valve plate.	Vibration signal analysis using wavelet analysis and Artificial Neural Networks.	No specific problems were mentioned, but spectral analysis and feature selection techniques is emphasized.	Develops a methodology to detect and classify wear faults in valve plates, facilitating condition-based maintenance.
[18]	Weak faults in hydraulic pumps.	Vibration signal fusion using Enhanced Empirical Wavelet Transform and Variance Contribution Rate.	Inadequate segmentation of the spectrum in the Empirical Wavelet Transform.	Introduces an improved method to achieve more accurate spectrum segmentation, enhancing weak fault detection.
[19]	Failures in positive displacement pumps, specifically in three-screw spindle pumps.	Extended Kalman Filter for the estimation of non-measurable signal data.	Difficulty in obtaining accurate mathematical models and the inability to use conventional sensors due to fluid turbulence.	Development and implementation of a prototype that improves accuracy and reliability in fault detection, providing a solution without the need for traditional sensors.
[20]	Abrasive wear in components of a positive displacement multi-piston pump.	K-Nearest Neighbor classifier based on vibration signals, static and dynamic pressure, and working medium flow rate.	Formation of elliptical depressions on the cam plate and microchannels in the valve plate due to the loss of the lubricating layer.	Demonstrates that a basic classifier like K-Nearest Neighbor can achieve high accuracy in detecting wear conditions.

[21]	Wear of the valve plate in a swash-plate axial piston pump.	Causation-based Linear Interpolation and Wavelet-based Adaptive Signal Analysis of Instantaneous Angular Speed Fluctuation waveform.	Interference of sensors position, periodic noise disturbances from bearings, shafts, and other rotating components.	Application of the Instantaneous Angular Speed signal for fault diagnosis of a swash-plate axial piston pump, for detecting wear faults in the valve plate. This approach is validated through experimental results.
[22]	Wear conditions and cavitation phenomena.	Support vector machines, extreme learning machines, deep belief networks and the minimum redundancy maximum relevance algorithm for feature ranking.	The limitation of conducting diagnostics under stationary operating conditions may not fully represent the operational realities of hydraulic systems.	Development of a neural classifier for pump wear state classification with high accuracy rates for pressure signals and the application of deep machine learning techniques to effectively detect and classify multiple faults in hydraulic systems.
[23]	The fault type analyzed is the detection of PDM (Positive Displacement Motor) stalls during coiled tubing operations.	Fuzzy Logic Inference System (FIS) that monitors surface parameters and detects motor stalling using data from coiled tubing unit surface sensors.	The limitation of a relatively small dataset available for development, which contains data from only 4 milling operations, and the reliance on human interaction with the equipment that is not recorded in the data.	The main contribution of the research is the development of a Fuzzy Logic Inference System that supervises surface data, recognizes abnormal situations, and informs the user to help avoid human-induced errors during coiled tubing operations.
[27]	Slight cylinder faults and severe cylinder faults in axial piston pumps.	The physics informed neural network framework is used for predicting pump flow ripple, which serves as a clear indicator of pump health. The study utilized a calibrated pipeline model to obtain simulated pressure ripples.	The time-consuming and expensive nature of solving the inverse problem, poor initial and partial boundary conditions.	Their framework has been validated through numerical and experimental studies, demonstrating high accuracy in predicting flow ripples and identifying fault characteristics, thus enhancing fault diagnosis in hydraulic systems.
[28]	Axial piston pump faults, including slipper wear, loose boot, and valve plate wear.	Domain adversarial transfer fault diagnosis method based on multi-scale attention mechanisms.	Insufficient feature extraction and domain adaptation capability in cross-situation and partially unlabeled samples.	The proposed method effectively improves fault diagnosis accuracy and provides new ideas for further research on axial piston pump fault diagnosis.

III. METHODOLOGY

To develop this work, a test bench (see Fig. 2) equipped with a Siemens 40 [HP] 1200 rpm electric motor and an Eaton 54 series axial piston pump was used to induce the failure conditions (see Fig. 3). The load was generated by means of a manifold consisting of two crossed relief valves, with which it was possible to maintain the same load conditions during the experiment (see Fig. 4).

Fig. 2. Test bench

Fig. 3. Positions taken for vibration measurement.

Two datasets were collected, one for normal and another for fault conditions test data are also separated to perform failure predictions under unknown conditions. At a pre-established load of 700 psi, maintaining the measurement variables such as operating regime, external noises, and hydraulic oil temperature in a constant range. To perform the proposed study, we proceeded to capture signals of preload pressure, discharge pressure, and mechanical vibrations in four points at the pump, in fault and non-fault conditions must be gathered (Table III).

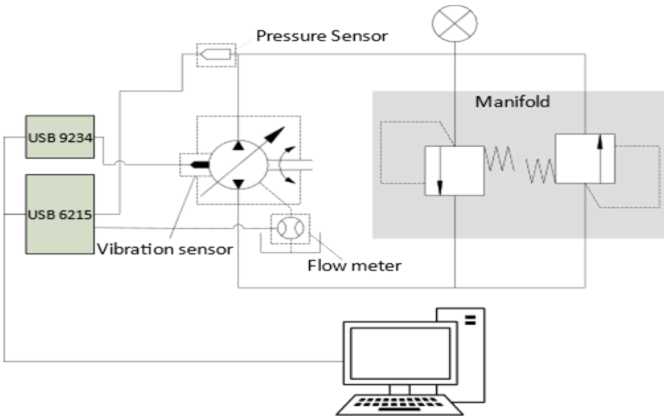

Fig. 4. Experiment's schematic.

Instrumentation and sensors:

- WIKA pressure transducer model ECO-1 to measure discharge pressure.
- Diagnostic systems for hydraulic systems based on signal analysis.
- Diagnostic systems for hydraulic systems based on knowledge or so-called intelligent fault identification.
- NI USB-6215 card
- NI USB-9234 card
- Laptop for data analysis.

TABLE III
PROCESS DATA CORRESPONDING TO NORMAL AND FAULT OPERATING CONDITIONS

Case	Vib 1	Vib 2	Vib 3	Vib 4	Precharge pressure Volt	Discharge pressure Volt
1	X_{11}	X_{12}	X_{13}	X_{14}	X_{15}	X_{16}
2	X_{21}	X_{22}	X_{23}	X_{24}	X_{25}	X_{26}
-	-	-	-	-	-	-
-	-	-	-	-	-	-
-	-	-	-	-	-	-
n	X_{n1}	X_{n2}	X_{n3}	X_{n4}	X_{n5}	X_{n6}

The experiment uses the components mentioned above and LabVIEW software for signal acquisition. The sampling frequency was 100 kHz for pressure data and 50 kHz for vibration data. Intentionally wearing out the valve plate induces one kind of fault condition: loss of volumetric efficiency. The data set includes data obtained when the pump worked in both fault and normal conditions and comprises 2^{16} observations from the six variables.

The Fast Fourier Transform (FFT) was applied to time series data to explore signals' spectral characteristics. The FFT decomposes vibration signals into their frequency components, enabling visualization of how fault conditions alter the data's spectral characteristics. The amplitude spectrum is calculated for each signal of each variable (sensor), highlighting frequency differences between normal and fault conditions.

In the Fig. 5. we can see the difference in the vibration spectrum in fault and not fault for the four accelerometer positions.

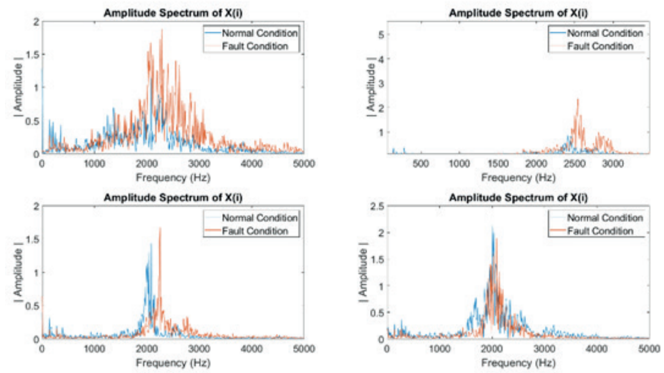

Fig. 5. Vibration Spectrum for normal and fault condition.

A. Principal Component Analysis (PCA)

PCA reduces data dimensionality and extracts the primary characteristics describing data variations. The technique projects data into a lower-dimensional space while preserving maximum variance [24]. Given a set of observations associated either with control, monitoring or simply as indicators of the process, new variables called principal components are constructed such that considering a data matrix $X \in R^{n\times m}$ (Eq. 1):

$$X = \begin{pmatrix} x_{11} & \cdots & x_{1n} \\ \vdots & \ddots & \vdots \\ x_{m1} & \cdots & x_{mn} \end{pmatrix} \tag{1}$$

It is convenient to normalise the data for each variable so that all the variables have the same weight in the computation. Then from this matrix, the covariance matrix can be calculated as follows (Eq. 2):

$$S = \frac{1}{n-1} X^t X \tag{2}$$

Performing singular value decomposition (SVD) (Eq. 3):

$$S = V \Lambda V^2 \tag{3}$$

Where Λ is a diagonal matrix with the eigenvalues of S sorted in descending order $(\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_m \geq 0)$, the columns of the matrix V are the eigenvectors of S. The transformation matrix $P \in \mathbb{R}^{m\times a}$ is generated by choosing the eigenvectors or columns V corresponding to the eigenvalues. For each dataset (normal and fault), the number of principal components necessary to explain at least 90 % of the variance is selected by the percentage of variability explained criterion, where the number of principal components a is taken so that P_a is close to a user-specified value [25], and the new dataset of smaller dimensions than the original is given by Eq. 4:

$$T = XP \tag{4}$$

Now, the original dataset can be represented in terms of its eigenvectors, which define the direction of the principal components (Eq. 5):

$$\widehat{X} = TP^T \tag{5}$$

The difference between the original dataset and the transformed dataset is the residue matrix (Eq. 6):

$$E = X - X^X \tag{6}$$

B. Statistics for monitoring with PCA

- Hotelling (T^2): This statistic is used to detect anomalies in new observations by comparing T^2 values to a determined threshold. Given an observation vector of the process, we can define this states statistic of the form (Eq. 7):

$$T^2 = X^T P \Lambda_a^{-1} P^T X \tag{7}$$

This threshold can be calculated from the sample data following Eq. 8:

$$T_a^2 = \frac{a(n^2-1)}{n(n-a)} F_\alpha(a, n-a) \tag{8}$$

Where n is the number of samples taken for the calculation of the PCA and F_a $(a, n – a)$ is the critical value of the Fisher-distribution) with n and $(n – a)$ degrees of freedom and a level of significance, which specifies the degree of commitment to false alarms. Its most typical values are 0.01 and 0.05.

C. Cluster analysis

According to [25], K-means clustering is an unsupervised non-hierarchical clustering algorithm focusing on similarity. It was applied to group data into two clusters: one for normal conditions and another for fault conditions. Once PCA has reduced the data, we apply the K-means clustering algorithm to group the data points into clusters to identify normal and fault condition data clustering patterns [26]. Given a set of observations (x_1, x_2, x_3,…, x_n) and ($S = S_1$, S_2, S_3,…, S_n) is the sum of the distances from the objects to its centroid and minimizing it; m_i is the mean (also called centroid) of points in cluster (Eq. 9).

$$\min \sum_{i=1}^{K} \sum_{x_j \in S_{\bullet i}} \|x_j - \mu_i\|^2 \tag{9}$$

Finally, we used silhouette analysis to evaluate the quality of the clusters obtained. According to [5] Data i in the cluster C_i, *a (i)* is the average intra-cluster distance and *(bi)* is the average inter-cluster distance. The number s(i) is obtained by combining a(i) and b(i) following Eq. 10:

$$s(i) = \frac{b(i) - a(i)}{\max\{b(i), a(i)\}}; -1 \leq s(i) \leq 1 \tag{10}$$

The silhouette coefficient measures the coherence and separation of the points within the clusters. However, instead of calculating the silhouette coefficient in the original data space, we calculate it in the principal component space. This allows us to visualize and evaluate the quality of the clusters in a lower-dimensional space. These plots assess cluster cohesion and separation, indicating the effectiveness of segmentation. The silhouette score measures how well samples are clustered with similar samples to evaluate the quality of clusters produced by clustering algorithms like K-Means [4]. The silhouette score can range from -1 to 1, with higher values indicating well-clustered objects and lower values suggesting that an object might belong to the wrong cluster.

D. Parameter Selection

The number of clusters (k=2) was determined for K-means clustering based on our prior knowledge of the system states (normal and fault conditions). For the silhouette analysis, a minimum silhouette score threshold of 0.5 was established to ensure cluster quality. For both analyses, the distance metric employed was “correlation,” which is defined by the Matlab Help Center as “One minus the sample correlation between points (treated as sequences of values).” In this context, each centroid represents the component-wise mean of the points within that specific cluster, following the procedure of centering and normalizing these points to achieve a zero mean and unit standard deviation. This approach ensures that the clustering process effectively captures the underlying relationships between data points while accounting for variations in scale and distribution.

IV. RESULTS

A.Data Preprocessing and Principal Component Analysis

The results of the PCA analysis indicated significant dimensionality reduction. The initial dataset, which comprised six variables, was effectively condensed into a lower-dimensional space. This reduction was achieved using three principal components, which collectively accounted for at least 90 % of the total variance, (see Fig. 6). This finding underscores the efficacy of PCA in simplifying complex datasets while retaining critical information.

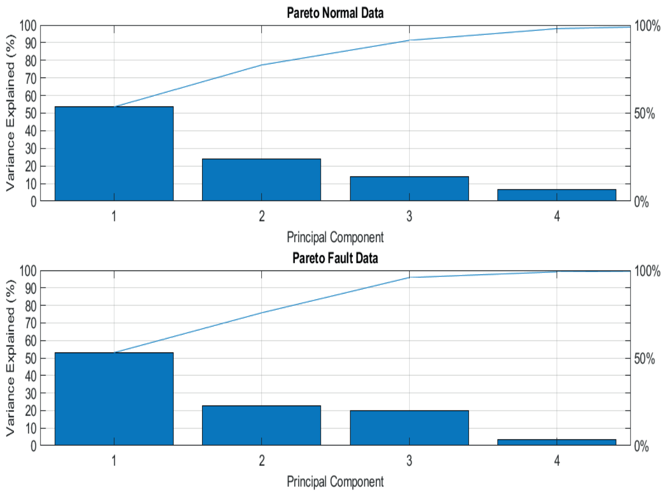

Fig. 6. Pareto

B. Clustering Results

K-means clustering was applied to the data transformed through Principal Component Analysis (PCA), successfully generating two distinct clusters. One cluster represents normal operational conditions, while the other encapsulates fault conditions. This method effectively separates the data points corresponding to normal and fault conditions, thereby enhancing the understanding of the underlying patterns within the dataset. Such differentiation is crucial for monitoring and diagnosing system performance in various applications (see Fig. 7). The Silhouette scores were computed within the principal component space, revealing strong indications of effective cluster separation and coherence. This analysis suggests that the clustering methodology employed is successful in distinguishing between the identified groups while maintaining internal consistency among observations within each cluster (see Fig. 8).

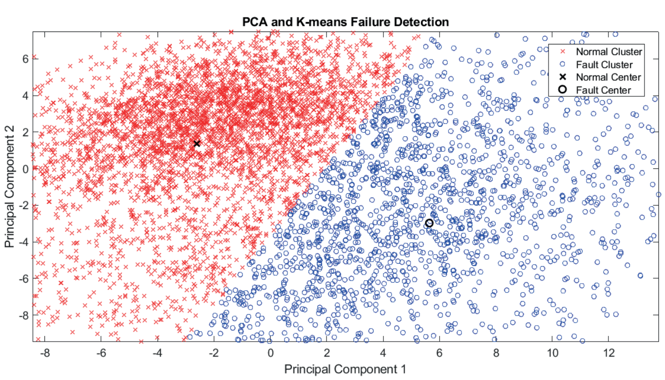

Fig. 7. Clusters from Normal and Fault data by K-means

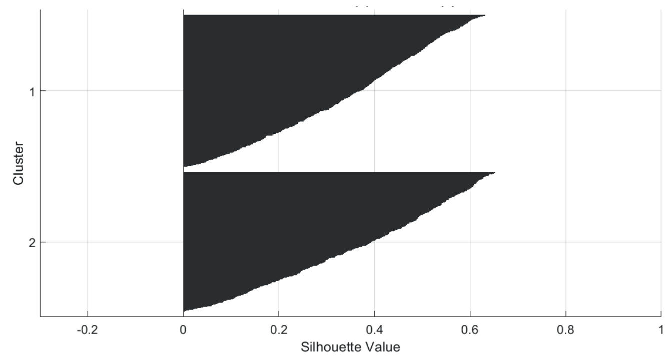

Fig. 8. Clusters from Normal (1) and Fault (2) data

C. Anomaly Detection Statistics

The T^2 statistic threshold was determined using the Fisher distribution (see Fig. 9). Observations that exceed this threshold were identified as potential anomalies, with significance levels set at 0.05. Figure 10 depicts the monitoring of the T^2 and how is able to detect the failure at the instant of occurrence (1000).

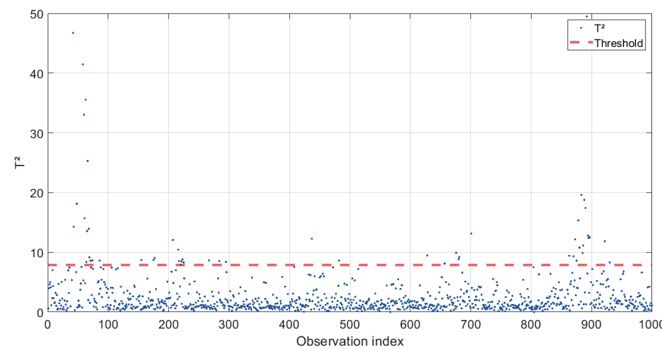

Fig. 9. Threshold

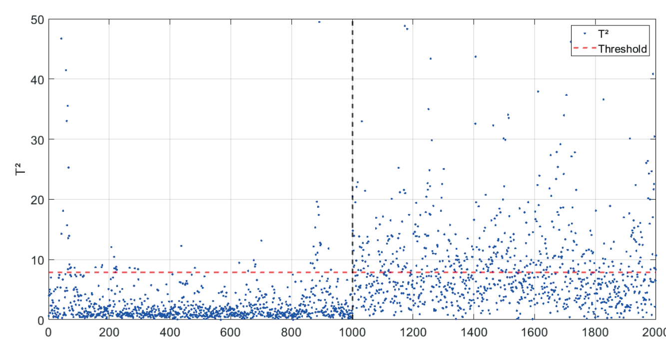

Fig. 10. Fault Detection

V. DISCUSSION

While our methodology has demonstrated promising results in fault detection, certain limitations must be acknowledged. Primarily, the approach tends to assume steady-state operational conditions, which may restrict its applicability in more dynamic environments characterized by rapidly changing system states. Moreover, although Principal Component Analysis (PCA) is effective for dimensionality reduction, it may unintentionally overlook complex nonlinear relationships present within the data. Additionally, the current clustering methodology necessitates complete retraining when encountering new fault types, which could hinder its adaptability and scalability across various hydraulic system configurations.

To mitigate these limitations, we could consider the integration of deep learning techniques to enhance the management of complex nonlinear relationships. Developing adaptive clustering parameters would facilitate a more dynamic assessment of different operating conditions. Furthermore, extending the method to accommodate multi-fault classification scenarios would significantly enhance its versatility in hydraulic systems.

Performing a comparative analysis. The proposed method of PCA and silhouette analysis offers advantages in terms of computational efficiency, interpretability of results and ability to operate without labeled data. However, it is limited by its dependence on linear relationships and requires careful parameter tuning. In contrast, deep learning techniques excel at capturing complex patterns and handling nonlinear relationships, but require large data sets and considerable computational resources. Fianlly, model-based approaches offer a unique perspective due to their physics-based understanding and ability to operate with limited data; however, they face challenges related to complex model development processes and system-specific constraints. These methodologies present a unique balance between computational complexity, data requirements, and diagnostic accuracy, demonstrating the importance of selecting an approach that fits the specific characteristics of the hydraulic system and the objectives of each investigation.

VI. CONCLUSION

The findings illustrate the effectiveness of this methodology in revealing clearer clustering patterns and helping to identify potential anomalies or deviations from standard operational conditions.

The proposed methodology effectively reduces the dimensionality of the data while preserving crucial essential information for fault detection. Silhouette analysis within the principal component space emerges as a valuable tool to assess and visualize the quality of the cluster, which aids in the identification of anomalies. The method shows promise for early fault detection by identifying possible transient states or emerging fault conditions.

Despite the encouraging results, further research is needed to validate the reliability of the method across various operating conditions and fault types. Future studies should incorporate systematic comparisons with other fault detection methods, investigate alternative clustering techniques, and validate the findings using a more diverse and extensive dataset.

Looking ahead, future work will focus on further exploring and refining this methodology across different domains and datasets, as well as investigating other techniques and algorithmic combinations to achieve even more robust results. Fault detection is a continually evolving field, and the use of combined approaches can enhance the accuracy and efficiency of these processes.

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Development and evaluation of the formulation of a biofertilizer based on the Anabaena-Azolla complex

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***Abstract* — Safety in agricultural production is one of the crucial parameters for fruits and vegetables, achieved through sustainable agriculture. In this study, the cyanobacterium Anabaena was evaluated in symbiosis with the plant Azolla sp, for the development of a biofertilizer. Samples were collected in Cusubamba, Pichincha, and seven culture media with different nutritional contributions were tested. In the Azolla study, the initial and final weights are analyzed to measure growth, the time to evaluate the development, and the cultivation area, which determines the area available for the determination of the biomass. These variables together allow the performance and sustainability of Azolla to be assessed. The best treatment was T2 (Nitrofoska 1g), achieving 66.59 g of fresh weight, a growth rate of 3.83 g/d, and a doubling time of 5.96 days. Dumas' method showed that T2 concentrated about 5% nitrogen. The biofertilizer complied with the characteristics and quality of the Phytosanitary and Zoosanitary Regulation and Control Agency (Agrocalidad-Ecuador), such as the absence of pathogenic microorganisms and the presence of macro and micronutrients such as nitrogen, which presented an average percentage of 1.54%, in addition to moderately optimal physical parameters such as a pH of 4.68 and a density of 0.016 g/mL.**

***Keywords*: Bioinput, Anabaena, Azolla, Cyanobiont, Nitrogen.**

***Resumen* — La seguridad en la producción agrícola es uno de los parámetros cruciales para las frutas y hortalizas, que se consigue a través de la agricultura sostenible. En este estudio se evaluó la cianobacteria Anabaena en simbiosis con la planta Azolla sp, para el desarrollo de un biofertilizante. Se recolectaron muestras en Cusubamba, Pichincha, y se probaron siete medios de cultivo con diferentes aportes nutricionales. En el estudio de Azolla se analiza el peso inicial y el peso final para medir el crecimiento, el tiempo para evaluar el desarrollo y el área de cultivo, que determina la superficie disponible para la determinación de biomasa. El conjunto de estas variables permite evaluar el rendimiento y la sostenibilidad de Azolla. El mejor tratamiento fue T2 (Nitrofoska 1g), alcanzando 66,59 g de peso fresco, una tasa de crecimiento de 3,83 g/d y un tiempo de duplicación de 5,96 días. El método Dumas mostró que el T2 concentraba aproximadamente un 5% de nitrógeno. El biofertilizante cumplió con las características y normas de calidad de la Agencia de Regulación y Control Fitosanitario y Zoosanitario (Agrocalidad-Ecuador), como la ausencia de microorganismos patógenos y la presencia de macro y micronutrientes como el nitrógeno, que presentó un porcentaje promedio de 1,54%, además de parámetros físicos moderadamente óptimos como un pH de 4,68 y una densidad de 0,016 g/mL.**

***Palabras clave:* Bioinsumo, Anabaena, Azolla, Cianobionte, Nitrógeno.**

I. INTRODUCTION

IN Ecuador, the agricultural sector is one of the most important productive axes because it occupies 24.29% of the country's total exports, in addition to contributing with participation the employment of around 26.8% of the economically active population (EAP). Agriculture, in turn, is a fundamental precursor of economic growth in developing countries such as Ecuador, so its contribution to the country's Gross Domestic Product (GDP) is 7.81%, which represents approximately 8,410.8 million dollars [1] [2].

Currently, agricultural systems in Ecuador present the need to improve their productivity and quality. Fertilization is a fundamental part of the production process, where the use of chemically synthesized fertilizers is common. Biofertilizers are an alternative to replace conventional fertilizers, as they allow the natural properties of crops to be maintained, without harming their cycles and preserving the fertility of ecosystems. In addition, biofertilizers facilitate the interaction between the existing microbiota in the crop and have the advantage of being made from microorganisms (bacteria, cyanobacteria, fungi, microalgae, or derivatives) which offer different benefits to crops, such as nitrogen fixation (N2), solubilization of phosphorus (P) and potassium (K), and assimilation of sulfur (S) [3] [4].

In agriculture, nitrogen is one of the macronutrients of greatest interest, it is used by the plant in the form of nitrate (NO3-) and ammonium (NH4+) for the optimal development of its vital processes. However, some agricultural producers use nitrogen fertilizers such as urea, excessively, forcing production without taking into account that the quality of the crop decreases due to poisoning by excess nitrogen. This also causes eutrophication, water toxicity, soil, and ecosystem degradation, contamination of groundwater flows, reduced biodiversity and biological imbalances [5].

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The *Azolla-Anabaena* partnership is presented as a viable alternative to reduce the adverse effects of the indiscriminate use of conventional agrochemicals, since it manages to fix atmospheric nitrogen (N2) and reduces it to ammonia, allowing the Azolla to assimilate nitrogen as a nutrient for its growth [4] *Azolla* spp. is a genus of floating aquatic ferns, which grow in bodies of fresh water, such as lagoons, lakes, or artificial reserves, and develop in tropical and warm areas, this fern can cover the entire surface of the body of water [6].

The leaves of the genus *Azolla* measure between 1 and 2 cm in diameter, and their color varies between reddish and greenish, with a circular or triangular shape. The adventitious roots can measure up to 30 mm in length and the stem, which is branched, is covered by small, alternate and lobed leaves, which consist of a submerged lower lobe (ventral) and an upper lobe (dorsal) that captures light energy, water and CO2 to carry out the photosynthesis process. In this upper lobe is a thin mesophyll filled with mucilaginous cavities that harbor the cyanobacterium *Anabaena azollae* [7].

Azolla reproduces in two ways: asexual and sexual; Asexual reproduction occurs through leaf fragments from lateral branches of the stem, where shoots grow spontaneously. Sexual reproduction is carried out using two types of floating spores: megaspores (female) and microspores (male), when fertilization occurs between the anterozoid that develops in the microspores (male gamete) and the egg (female gamete) [8].

Another organism that is part of the symbiosis is the filamentous cyanobacterium *Anabaena azollae,* whose hue is bluish-green and has chlorophyll a. This photosynthetic microorganism grows symbiotically extracellularly in the cavities of the dorsal lobes of aquatic ferns in the Azolla to harness photosynthetic energy and fix atmospheric nitrogen. In the filaments of Cyanobacteria, there are cells called heterocysts, which comply with the fixation of N2 [9].

Anabaena azollae is a photosynthetic cyanobiont that has vegetative cells in the apical meristem of the Azolla sporophyte, the differentiation of heterocysts occurs with the development of the leaf cavities. Cyanobiont has a gram-negative cell wall, cytoplasmic inclusions, and a simple thylakoid system. The heterocyst has cyanoffice nodes, a thick wall, and honeycomb thylakoids [10].

According to *to Anabaena* sp., it is a cyanobacterium that reproduces mainly by fragmentation by hormogonia. Hormones are specialized filaments or cell chains that separate from the parent colony and can mobilize to establish and colonize new areas, developing and forming new cyanobacteria [10].

In the symbiosis between the cyanobacterium Anabaena and the Azolla plant, contact is established when the Azolla sporophyte breaks the apical membrane, initiating the symbiosis. Anabaena concrete differentiates into akinetes in the megasporocarp, remaining dormant until the plant germinates, restarting the symbiotic cycle [11].

The growth conditions of the symbiosis can be categorized into two factors, as shown in Table I: physical and climatic factors, and chemical factors. It should be noted that in addition to the nutrients mentioned in the [10] [11], azolla also requires magnesium and sulfur, as well as minimal amounts of micronutrients such as zinc, manganese, copper, chlorine, and molybdenum.

TABLE I
GROWING CONDITIONS

Physical and climatic factors		**Chemical factors**	
Environmental Temperature	18 to 28 ºC	pH	5 a 7,5
		Nitrogen (N)	3 a 10 Kg N/ Ha
Water Temperature	5° to 35°C	Phosphorus (P)	2 to 4 ppm
Light	1500 lux	Calcium (Ca)	11 to 28 ppm
Relative humidity	70 to 75%	Potassium (K)	1 to 5 ppm
Water Depth	>3cm	Iron (Fe)	1 ppm

For the overcrowding of Azolla, it is important to bear in mind that, according to [12], this fern can double in weight in a period of 6 to 15 days. Starting from an initial amount of 0.16 kg, the biomass increased by 5.63 kg over a period of 19 days. Therefore, determining the appropriate culture medium is essential, since the amount of biomass obtained depends on the nutrients present in the medium.

For good massification and adequate development of symbiosis, the use of culture media that includes elements such as cow, horse or poultry manure (a source of nitrogen) is recommended. In addition, it is advisable to complement these with commercial media such as BG11, a culture medium for cyanobacteria that has macro and micronutrients or Nitrofoska which is a fertilizer used in agriculture rich in macronutrients [13].

The *Anabaena-Azolla* complex can fix about 200 kg of nitrogen (N) per hectare per year. This process is carried out thanks to the heterocysts of the Anabaena symbiont, where the nitrogen-fixing enzyme, nitrogenase, is located *Anabaena azollae* reduces the molecule from nitrogen (N2) to ammonia (NH3), as can be seen in Equation (1), proposed by [14].

$$N2 + ATP \rightarrow (nitrogenase) \rightarrow 2\,NH3 + 12ADP + 12Pi. \quad (1)$$

The FBN (Biological Nitrogen Fixation) in *Anabaena azollae* is intimately related to photosynthesis, which provides the ATP and reductant needed to convert nitrogen to ammonia in symbiosis. Three key enzymes in the assimilation of ammonium are glutamine synthetase, glutamate synthetase and glutamate dehydrogenase. Glutamine synthetase, present in the heterocyst, incorporates nitrogen fixed in glutamine, while glutamate synthetase acts in vegetative cells, transporting glutamate to heterocysts. The fixed nitrogen is transported to the host, where it is integrated into amino acids, which, together with the reductant and photosynthate, are supplied to the symbiont [15].

Anabaena azollae not only fixes nitrogen, but also excretes ammonia, cyanobacteria promote the use of N2 to determine the distribution of nitrogenous compounds produced by symbiosis with Azolla, activity that was evidenced in [16], where it was determined that N2 was distributed as extracellular ammonia (49.9%), intracellular ammonia (6.4%), extracellular organic nitrogen (5.6%), and intracellular organic nitrogen (38.1%).

It is important to mention that, in the nitrogen cycle, during the assimilation phase, plant roots take ammonia (NH3), ammonium (NH4+), and nitrate (NO3–) to integrate them into the process of chlorophyll formation, leaf development, photosynthesis, and protein synthesis [17].

In Ecuador, this symbiotic complex has been used mainly in rice crops as an organic fertilizer. Due to the ability of the *Anabaena-Azollae* symbiotic complex to fix atmospheric nitrogen (N2), this partnership could be an alternative for the production of biofertilizers that meets the bio input control requirements of Ecuador regulated by the Agency for Phytosanitary and Zoosanitary Regulation and Control (Agrocalidad) under resolution 218, section X, specific requirements for the registration of biological inoculants for the registration of fertilizers an inoculum of nitrogen-fixing bacterial strains, whose relevance prevails in the control and registration of related products for agricultural use in Ecuadorian territory, by its requirements and procedures for correct control of fertilizers, soil amendments and related products for agricultural use [18].

This research was carried out in the laboratories of the Agency for Phytosanitary and Zoosanitary Regulation and Control (Agrocalidad), Tumbaco, for a period of ten months. The objective was to develop and evaluate the formulation of a biofertilizer made from the *Anabaena-Azolla* symbiotic activity, through massification in different Azolla culture media. This included identifying and characterizing *Anabaena–Azolla m*icroscopically, quantifying biomass and nitrogen content, analyzing growth rate, and evaluating the biofertilizer's physical, microbiological, and micro/macronutrient properties. The study ensured compliance with the quality control parameters outlined in resolution 218 of Agrocalidad for agricultural inputs and derivatives with nitrogen (N2) content.

II. MATERIAL AND METHODS

A. Harvesting of plant material for cultivation

The plant specimens of *Azolla* spp. were collected in Santa Rosa de Cusubamba (-0.028416, -78.283000), altitude: 2694 m.a.s.l., located in the province of Pichincha, Cayambe canton, with the help of 307.87 (L) plastic buckets and shovels for the collection of plant samples.

B. Suitability of culture media for the Azolla massification phase

The specimens were cultured in plastic containers 40 cm long by 25 cm wide, applying the A total of seven culture media, referred to as treatments (T), were tested along with one control (T8) Table II. The specimens were cultured in plastic containers measuring 40 cm in length and 25 cm in width. A total of seven culture media, referred to as treatments (T), were tested, along with one control (T8), as shown in Table II. Each of these contained 4 L of water with its respective components. 13 g of fresh Azolla was added as the initial inoculum in each of the treatments for massification; in these mass media, certain treatments containing commercial media were carried out such as Hoagland which is a hydroponic culture medium used for the growth of plant species, Nitrofoska whose nutritional content is nitrogen, phosphorus and potassium, BG11 which is a liquid culture medium for algae growth [17].

TABLE II
TREATMENTS FOR AZOLLA MASSIFICATION

Treatment	Description of compounds and quantities
T1	Soil (200g) + Manure (250g)
T2	Nitrofoska (1g)
T3	Soil (200g) + Manure (250g) + BG11 (100mL)
T4	Soil (200g)
T5	Soil (200g) + Manure (250g) + Nitrofoska (1g)
T6	Soil (200g) + Manure (250g) + Hoagland (100mL)
T7	BG11 (100mL)
T8	Irrigation water (control) (4L)

C. Identification of Anabaena azollae

Before massification, the cyanobacteria of interest were observed under a microscope. To do this, 1 gram of *Azolla was* weighed, macerated in 9 mL of distilled water, and a drop of the dilution was placed on a slide, which allowed the identification of cyanobacteria and their structures, such as heterocysts [18].

D. Experimental design of culture media

For the statistical analysis of the Azolla culture media, a Completely Randomized Design (DCA) was used with 3 blocks that were defined by the three different harvest times, with periodic evaluations of 14 days. At the end of each period, the biomass obtained was weighed and a 13 g inoculum was placed for a new reproduction of Azolla. The resulting biomass was dried in an oven for 24 h at temperatures ranging from 40 ºC to 50 ºC to later quantify the total nitrogen [18].

E. Azolla Biomass

To measure biomass growth in dry and fresh weight, the mean absolute growth rate (MAGR) (Equation 2), the average crop growth rate (ACGR), which is the growth of the plant per square meter per day (Equation 3), the average relative growth rate (ARGR), which represents that for each gram of Azolla base how many grams grow per day (Equation 4) and the doubling time (DT) (Equation 5). These quantitative analyses use data such as dry weight (W2), fresh weight (W1), time (T) and other variables such as the area of the container, which is determined by multiplying the length by the width (Equation 6), these data allow interpreting and describing the growth of plants in semi-natural environment conditions [19].

$$MAGR = \frac{W2-W1}{T} = g/day \ (2)$$

$$ACGR = \frac{W2-W1}{Container\ area} = g\ m^2/day \ (3)$$

$$ARGR = \frac{Log_{(e)}(W2)-Log_{(e)}(W1)}{T} = g * g/day \ (4)$$

$$DT = \frac{ln_2}{ARGR} = days \ (5)$$

$$Vessel\ area = Length\ (x)\ Width \ (6)$$

F. Dumas Nitrogen Quantification

The percentage of total nitrogen (%N) at the Azolla plant was quantified using the Dumas combustion method. To do this, 1.5 mg of the dry and pulverized sample was weighed, placed on aluminum foil and fed into a nitrogen analyzer. The sample is burned at 1000 ºC in the presence of pure oxygen, generating a gaseous mixture. This mixture was conducted in a reduction chamber with hot copper, where the nitrogen oxides were converted into molecular nitrogen. Finally, water and carbon dioxide were removed, determining the percentage of total nitrogen using a thermal conductivity detector [20].

G. Biofertilizer formulation

The composition of the biofertilizer included *Azolla* spp. In addition, excipients were used. The biofertilizer was formulated in the liquid base from the harvest of azollas, they were drained in a sieve to remove excess water from the medium and then 50 g were weighed to mix them in 500 mL of boiled water, the solution was homogenized with a blender, then 1.5 g of citric acid was weighed. Which has preservative properties to improve the quality of the product by preventing contamination by microorganisms. For the other phase of the formulation, 1% carboxymethylcellulose (CMC) was placed in 500 mL of tap water, the function of the CMC was to retain the water [21] [22], then the solution was constantly stirred on a heating plate at 360 rpm until it dissolved completely and no lumps were observed, followed by this it was mixed with Azolla on the base solution (water and thickener) in constant agitation, until the bio preparation is homogenized [22].

H. Microbiological Testing

For the determination of the presence of microorganisms such as *E. coli, Staphylococcus aureus, Salmonella* Spp *Shigella* spp. and total coliforms, the proposed protocol was applied, where a dilution of 25 mL of the liquid biofertilizer was carried out in 225 mL of buffered peptone water, previously sterilized, and 15 minutes waited for the microorganisms to be incorporated into the environment. 100 uL of the previously prepared dilution was taken with the help of a micropipette and seeded in the following culture media: Titan Media brand methylene blue eosin agar (EMB) and BD brand Salmonella-Shigella selective culture medium. The dilution placed in each culture medium was dispersed with a sterile loop around the petri dish. 1 mL of the sample dilution was also placed in 3M Petrifilm™ plates for Staph Express Counting and the culture media were incubated for 24 hours at 36 ºC. After this time, the presence of the corresponding microorganisms was determined, if they were present, they were quantified by determining the colony-forming units (CFU) obtained by multiplying the number of colonies by the dilution factor (Equation 7), and the interpretation of the results was made based on the Table III.

$$\frac{CFU}{g} = \frac{Number\ of\ colonies\ x\ dilution\ factor}{mL\ of\ the\ sown\ sample} \quad (7)$$

TABLE III
INTERPRETATION OF THE PRESENCE OR ABSENCE OF MICROORGANISMS IN THE CULTURE MEDIA

Culture medium	**Microorganism**	**Colony**	**Presence or absence**
Agar EMB	*E. Coli*	Bright green	Presence, LMP 1000 CFU ($^{w-1}$)
	Total coliforms	Purple	
Petrifilm Plates	*Staphylococcus aureus*	Blue dots or parts	Absence
Agar *Salmo-nellaShigella*	*Salmonella* spp.	The color is black due to hydrogen sulfide	
	Shigella spp.	Transparent with green center	

For microbiological analysis of microorganisms such as *Listeria monocytogenes* and *Salmonella* spp., 500 uL of the LMX SUPP supplement was placed in 225 mL of *Listeria monocytogenes* Xpress (LMX) broth to prevent the growth of other microorganisms, stirred and transferred 25 mL of the biofertilizer sample. The solution was incubated at 41.5 ºC.

In 25 mL of the sample, 225 mL of buffered peptone water was added and mixed. Subsequently, 1 mL of the 3M *brand Salmonella* supplement (SUPP) was added and incubated for 24 hours at 37 ºC. The two corresponding solutions were placed in wells of different stream plates, taken to a thermoblock at 95ºC and placed in the mini VIDAS equipment of the bioMérieux brand, which through the ELFA method (Enzyme-Linked Fluorescent Assay), antigens of bacterial microorganisms are detected. This equipment specifies that when the index value (VT) is <1 it is negative and when it is >1 it is positive [23].

I. Micronutrient and macronutrient analysis

Macronutrients such as potassium and phosphorus, and micronutrients such as zinc, sodium, iron, copper, and manganese, were quantified by atomic flame spectrophotometry. The methodologies used are endorsed by the Agency for Phytosanitary and Zoosanitary Regulation and Control (Agrocalidad): for macronutrients and for micronutrients under the document that defines the methodologies based on [23].

The methods established by the AOAC were considered to define the respective concentrations of each of the aforementioned elements for the reading of macro and micronutrients through the use of an atomic absorption spectrometer.

III. RESULTS AND DISCUSSION

A. Identification of Anabaena under the Microscope

Cyanobacteria *Anabaena azollae* They were recognized by the presence of heterocysts, which are yellow and round in shape, compared to vegetative cells that are oval-shaped [24] (Fig. 1).

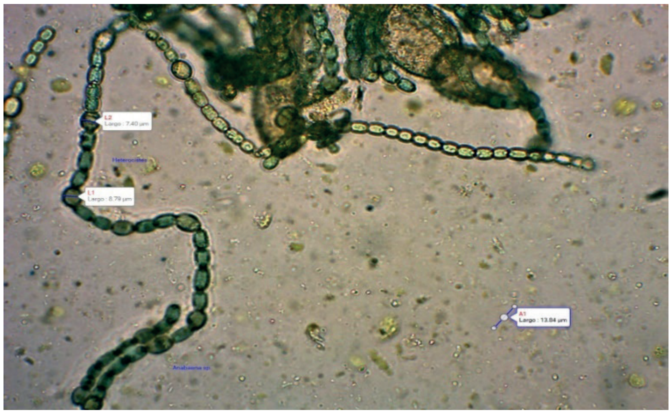

Fig. 1. Identification of *Anabena azollae.*

B. Massification of Azolla in culture media

From the initial inoculum, the first harvest was obtained after 15 days, it was determined that the Azollas of T4 (soil 200g) had long, reddish-brown roots and did not reproduce properly, since, according to the culture medium, it did not have enough supply of phosphorus, since the black soil did not contain enough of this nutrient [25].

In the second harvest, it was evident that the aquatic ferns adapted better to the treatments T1 (Earth (200g) + Manure (250g)), T2 (Nitrofoska (1g)), T3 (Earth (200g) + Manure (250g) + BG11 (100mL)), T5 (Earth (200g) + Manure (250g) + Nitrofoska (1g)) and T6 (Earth (200g) + Manure (250g) + Hoagland 100mL), since the massification time was faster unlike the first harvest, this is since studies such as the adaptation of the cyanobacteria to different conditions depend on components such as the production of redoxins in which glutarredoxins and thioredoxins are included, which are linked to the photosynthetic flow and nutrients that determine the expression of adaptability genes to the environment depending on the presence or absence of nitrogen in the environment [25]

In the third harvest, it was determined that the plants of the T1, T2, T3, T5 and T6 treatments have a complete adaptability to the culture media compared to other crops, as they obtain greater massification, with T2 being the one that generated a higher fresh weight as can be seen in Table IV.

C. Biomass and % nitrogen

The production of biomass and percentage (%) of nitrogen are positively correlated with the time of adaptability to the environment, since when observing the results concerning the blocks of time, the production of the aforementioned variables increases with respect to time, this is related to what was mentioned by those who describe that the Azolla together with the [26] *Anabaena azollae* it has the ability to adapt in the culture medium with respect to a period of time, as a consequence of the production of genes and proteins of the GS-GOGAT system (Glutamine synthetase-glutamate synthase) that when the nitrogenous conditions are rich activate all the nitrogen assimilation systems in the cells of the cyanobacteria, thus achieving ~~a~~ better assimilation of nitrogen and promoting the increase of biomass. Table V [27].

1. Biomass weights and percentage of Nitrogen

Fresh weight showed a significant difference with a p-value <0.0001, which means that at least one treatment is different. The T2 treatment (Nitrofoska 1g) obtained the highest average with a fresh weight of 66.59 g, as it can be interpreted that this fertilizer provides a base of selective nutrients to the medium so that the symbiotic association can increase its biomass [27]. On the other hand, the T8 treatment (control) obtained the lowest mean of 16.38 g. The T2, T3, T5, T1 and T6 treatments showed good biomass development because macronutrients such as K, N and P allowed biomass to double around 7 to 8 days (Table IV). Once the 3 harvests were concluded, it was determined that the Azollas can contain between 1 to 5% of the nitrogen. The nitrogen content can range from 1% to 5% in its dry matter, although some studies have reported figures that can vary between 2% and 7% depending on growing conditions and the specific species of Azolla [28].

The dry weight showed a significant difference with a p-value of 0.0034. The T3 treatment (soil + manure and BG11) obtained the highest mean of 2.03 g. This may be because the BG11 component contains Potassium Nitrate KNO3 as an active ingredient and its function is to allow the proliferation of cyanobacteria [29]. The T2 (Nitrofoska) and T5 (soil + manure + Nitrofoska) treatments also presented similar statistical results 1.88 to T3 for obtaining dry biomass by obtaining 1.91 g and g respectively [30]. The T8 treatment (control) had the lowest mean of 0.60 g.

In the analysis of treatments for the nitrogen percentage variable, using the DUMAS method, a significant difference was evidenced with a probability value p<0.05 of 0.0001. The T2 treatment (Nitrofoska), which showed 5.27% N, was the treatment with the highest percentage of nitrogen, this may be because Nitrofoska has essential nutrients such as nitrogen, phosphorus and potassium, to stimulate the growth of the azollas through the production of redox ins that increase the rate of photosynthetic electrons, which determines the expression of genes and regulation of different proteins to prioritize the absorption of nitrogen [31] On the other hand, the T4 treatment, which did not include additional supplements such as Nitrofoska or BG11, showed the lowest percentage of nitrogen, with 1.97%N.

TABLE IV
FRESH WEIGHT, DRY WEIGHT, NITROGEN PERCENTAGE OF TREATMENTS WITH TUKEY TEST (5%)

Treatment	Fresh weight	Dry Weight	% of N
T2	66,59 ± 5, 83 (a)	1,88 ± 0,81 (ab)	5,27 ± 0,10 (a)
T3	60,15 ±6,37 (ab)	2,03 ± 0,43 (a)	2,85 ± 0,12 (c)
T5	60,11 ± 6,67 (ab)	1,91 ± 0,39 (from)	3,17 ± 0,42 (bc)
T1	53,46 ± 15,78 (abc)	1,71 ± 0,17 (abc)	3,17 ± 0,28 (bc)
T6	46,81 ± 14,72 (abc)	1,53 ± 0,23 (abc)	2,88 ± 0,29 (c)
T4	36,97 ± 1,79 (bcd)	1,26 ± 0,35 (abc)	1,97 ± 0,34 (d)
T7	35,2 ± 1,16 (cd)	0,85 ± 0,27 (bc)	3,66 ± 0,12 (b)
T8	16,38 ± 2,07 (d)	0,6 ± 0,16 (c)	2,21 ± 0,44 (d)

TABLE V
TUKEY TEST (5%) FOR TIME LAPSES
IN PERCENT NITROGEN (%N) (BLOCKS)

Time	Mean ± D.E.	Rank
3	3,41 ± 0,94	a
2	3,03 ± 1,05	b
1	3,00 ± 1,08	b

D. Growth rate and doubling time analysis.

In this analysis, the data provided for the increase in biomass, time, area, length and width of the container is taken into account to develop the formulas for each of the treatments.

1. Mean absolute growth rate (MAGR)

In the absolute growth rate, the increase in Azolla biomass per day seem in the Fig. 2 (g/d).

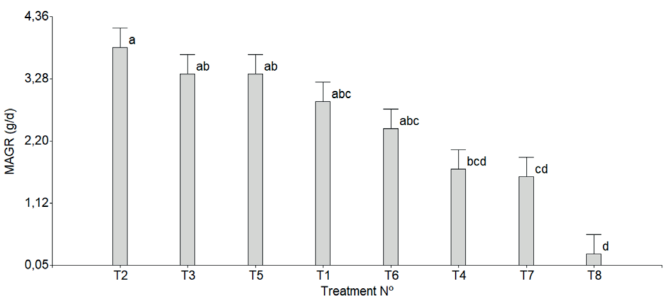

Fig. 2. Absolute growth rate of azollas.

It can be identified that treatments T2 (a), T3 (ab) and T5 (ab) are those with the highest growth rate with values corresponding to 3.83 (g/d), 3.37 (g/d) and 3.36 (g/d) respectively. The use of manure, such as goat and poultry manure, has shown positive results in the growth of Azolla, In addition, other elements such as Nitrofoska or BG11 provide essential nutrients that favor growth and nitrogen fixation by the symbiosis with Anabaena [30] [31].

2. Average Crop Growth Rate (ACGR)

As for the growth that was obtained per square meter per day (g.m2/d), in the Fig. 3 the bar graph for Tukey's test (5%) is presented.

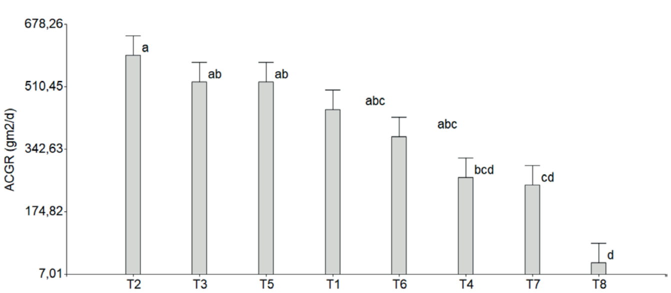

Fig. 3. Growth rate of azollas culture.

It can be observed that treatments T2 (a), T3 (ab) and T5 (ab) with means of 595 (gm2/d), 523.93 (gm2/d) and 523.40 (gm2/d) respectively, are the highest TMCC taking into account the short time in which biomass production is generated in the container area by the reason of partial shade is provided. especially to prevent the drying out of pteridophytes at midday [32].

3. Average Relative Growth Rate (ARGR)

In the TMCR, the growth is for each gram of base, how many grams the biomass of the symbiotic complex grows per day (gg/d) (Fig. 4).

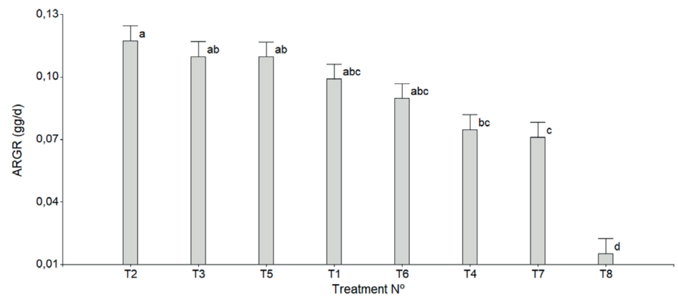

Fig. 4. Average relative growth rate of azollas

The treatments with the highest average are T2 (a), T3 (ab) and T5 (ab), with data corresponding to 0.12 (g.g/d) and 0.11 (g.g/d) for T3 and T5 treatments, since biomass production is distinctively high in 3 of the treatments, however, T8 shows a much lower growth [33].

4. Doubling Time (DT)

The variable (DT) allowed us to determine specifically in what time the biomass of the symbiotic complex begins to double in days (d) (Fig. 5).

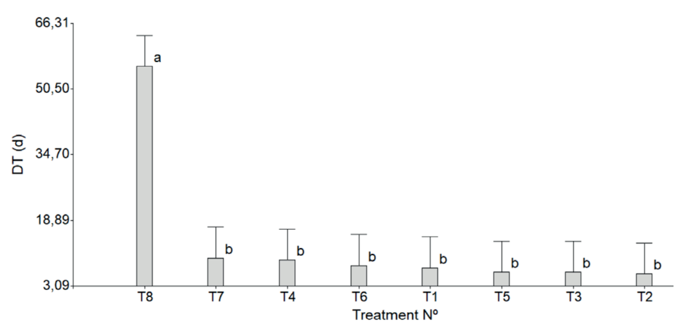

Fig. 5. Doubling time of the azollas

The treatment that requires the longest time to duplicate is T8, which in this case is precisely the control, while the treatments with the shortest doubling time are T2 (b) with 5.96 (d), T3 (b) and T5 (b) with 6.37 (d). It should be noted that the doubling time ranges from 5 days to 9 days in the case of treatments with the incorporation of culture media [34].

E. Physical analysis of the bioinput

1. Hydrogenic potential (pH)

The pH of the biofertilizer in its pure state was 4.68, however, when diluted in water in a ratio of 5 to 1, it tends to raise its pH to 6. The optimal pH present in a foliar input ranges from 5 to 6.5 [35].

2. Density

In the pycnometer a density of 1.016 g/mL was recorded, however, the most suitable density in a foliar fertilizer is around 1.20, the density obtained was low because there is more water in the fertilizer [36].

F. Microbiological analysis of the bioinput

The bioinput complied with the quality control parameters in force in resolution 218 of Agrocalidad for organic fertilizers, since each of the microbiological tests yielded negative results. There was no presence of bacteria such as *E. coli,* total coliforms, *Shigella* spp., *Salmonella* spp. and *Staphylococcus aureus* [37].

For the bacteria *Salmonella* spp. and *Listeria monocytogenes*, the mini VIDAS team yielded negative results for the bioinput, for *Salmonella* spp. The result was a VT of 0.05 and in relation *to Listeria monocytogenes*, a VT of 0.00 was obtained.

G. Micro and macronutrient analysis

The analysis of macro and micronutrients using the Dumas method allowed us to determine their corresponding percentages. Three analyses of the bioformulation were carried out: at the time of obtaining the bioproduct with a difference of 15 days between each analysis, where T0, T1 and T2 correspond to each of the repetitions performed.

TABLE VI
PERCENTAGE OF LIQUID MACRO AND MICRONUTRIENTS PRESENT IN LIQUID BIOFERTILIZER

Macronutrients	**T0**	**T1**	**T2**
Nitrogen (N)	1,54	1,52	1,56
Phosphorus (P)	1,4939	1,4941	1,4942
Potassium (K)	1,107	1,103	1,109
Calcium (Ca)	1,5026	1,502	1,5021
Magnesio (Mg)	1,4981	1,4978	1,4983
Micronutrients	**T0**	**T1**	**T2**
Zinc (Zn)	1,035	1,035	1,035
Sodium (Na)	1,5219	1,5216	1,5219
Iron (Fe)	1,4904	1,4904	1,4902
Copper (Cu)	1,053	1,051	1,061
Manganeso (Mn)	1,098	1,10	1,096

Nitrogen, with an average of 1.54%, was identified as the most abundant element in the formulation of the bioinput like seem in the Table VI, thanks to the activity of the heterocysts of *Anabaena azollae.* It was evidenced that the amount of macronutrients and micronutrients did not vary with respect to time, if the formulation is left in conditions of humidity and extreme temperature, the nitrogen could volatilize [37].

III. CONCLUSIONS

The best treatments were T2 (Water (4L) + Nitrofoska (1g)), T3 ((Water (4L) + Soil (200g) + Manure (250g) + BG11 (100ml)) and T5 ((Water (4L) + Soil (200g) + Manure (250g) + Nitrofoska (1g)). The T2 treatment stood out for generating an average fresh biomass of 66.59 g and a dry weight of 1.88 g. In addition, it presented the highest percentage of nitrogen with 5.27%.

T2 also showed a high growth rate with a MAGR of 3.83 g/d, a ARGR of 0.12 g.g/d, and a ACGR of 595 g*m²/d. Its doubling time was 5.96 days, which favors a rapid production of biomass.

The control parameters were evaluated according to Agrocalidad regulation 218, determining that the physical parameters were moderately adequate such as a pH of 4.68 and a density of 1.016 g/mL. Microbiologically, the biofertilizer complied with the regulations, since the absence of pathogenic microorganisms such as total coliforms, *E. coli, Staphylococcus aureus, Salmonella* spp. and *Shigella spp. was observed* , which indicates the excellent state of the bioinput.

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Artificial Neural Networks in the Oil and Gas Industry: Bibliometric Analysis (2020-2024)

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Abstract — **In the oil and gas industry, applying prediction and estimation methodologies such as Artificial Neural Networks has represented a valuable tool in the whole petroleum system. The review's objective was to analyze, from a bibliometric perspective, the scientific production of the last five years on the use of Artificial Neural Networks in this industry. The Scopus database was used to filter the information by time, subject, type of documents, and origin. A search equation was used with the keywords artificial neural network and oil and gas industry. The information was processed using LibreOffice Clac, JASP, and VOSviewer software. A total of 267 documents were obtained, with 59.9% original scientific articles, 56.0% published in scientific journals, China as the country with the highest production, the main authors were from Saudi Arabia, 69.8% of the research was in the Energy sub-area, 67.1% of the research was affiliated to oil companies and the application areas were, in addition to the traditional exploration, drilling, production and reservoir, flow analysis, artificial lift, emissions, anomaly detection, automation, corrosion, and carbon dioxide detection. It is concluded that in the last five years, research on the use of ANNs in the oil and gas industry has deepened, especially in production prediction, reserves, and reservoir studies.**

Keywords: **Artificial Intelligence; Artificial Neural Networks; Petroleum Operations; Predictions; Natural Gas; Bibliometrics.**

Resumen — **En la industria del petróleo y gas la aplicación de metodologías de predicción y estimación como las Redes Neuronales Artificiales ha representado una herramienta valiosa en todo el sistema petrolero. El objetivo de la revisión fue analizar, desde la perspectiva bibliométrica, la producción científica de los últimos cinco años sobre el uso de las Redes Neuronales Artificiales en esta industria. Se utilizó la base de datos de Scopus, filtrando la información por tiempo, temática, tipo de documentos y origen. Se utilizó una ecuación de búsqueda con palabras clave artificial neural network y oil and gas industry. La información se procesó mediante los softwares LibreOffice Clac, JASP y VOSviewer. Se obtuvo un total de 267 documentos, de los cuales el 59,9% correspondió a artículos científicos originales y el 56,0% fueron publicados en revistas científicas. China se posicionó como el país con mayor producción, mientras que los principales autores procedieron de Arabia Saudita. El 69,8% de las investigaciones se enfocaron en la subárea de Energía, y el 67,1% estuvieron afiliadas a empresas petroleras. Las áreas de aplicación incluyeron, además de las tradicionales (exploración, perforación, producción y yacimientos), el análisis de flujo, levantamiento artificial, emisiones, detección de anomalías, automatización, corrosión y detección de dióxido de carbono. Se concluye que, en los últimos cinco años, se ha profundizado la investigación sobre el uso de las RNA (redes neuronales artificiales) en la industria del petróleo y gas, especialmente en temas como la predicción de producción, reservas y estudios de yacimientos.**

Palabras clave: **Inteligencia Artificial; Redes Neuronales Artificiales; Operaciones petroleras; Predicciones; Gas Natural; Bibliometría.**

I. INTRODUCTION

TECHNOLOGICAL evolution has penetrated all levels of humanity's daily activities, and the oil and gas industry is no exception, especially the oil and gas industry, which is considered the main industry in the world energy market, due to the importance of hydrocarbons as a primary energy source [1].

Artificial Intelligence (AI) has been progressively used in industry as a means to optimize operations, increase productive capacity, and control pollutant emissions, ensuring product quality, in what has been called Industry 4.0 [2]. This is a fact also in the oil and gas industry, where the inclusion of AI tools such as Machine learning and Artificial Neural Networks (ANN) have proven useful in predicting the behavior of key parameters in processes and optimizing operations [3], [4].

Although review papers have been developed on the evolution of the use of AI in the oil and gas industry and how it has impacted all areas that compose it [5], these have focused on the technology in a general way, i.e., the use of any of the available AI tools or techniques. In the specific case of the use of ANN, research papers have been presented focused on solving operational problems and predicting conditions at different stages of the petroleum system [6], but there have been few reviews leading to an understanding of the evolution and importance given to ANNs in this industry, limited to reviews in specific areas such as in exploration [7], petrophysical properties [8], or reservoir characterization [9]. Some reviews have been more general in using ANNs [10].

Within the studies dedicated to the analysis of scientific production in a specific subject, bibliometrics is a popular and rigorous method for exploring and analyzing large volumes of scientific data, which allows for unraveling the evolutionary

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nuances of the subject, while giving a clear idea about the emerging areas in the same [11]. Thus, the use of bibliometric studies makes it possible to identify emerging trends in the production of scientific papers and the most important publication media, collaboration patterns, and research components, as well as to explore the intellectual structure of a specific field in the existing literature at a global level [12].

In the case of bibliometric studies referring to the use of AI, research in various areas of knowledge stands out, such as in health care [13], environmental operations [14], marketing [15], supply chains [16], among others. In the oil and gas industry, bibliometric analysis in sustainable production [17], in machine learning methods [18], and in general, the use of AI in petroleum engineering [19], and on trends and patterns of AI in the oil and gas industry [20].

Since few bibliometric studies have been visualized on the use of AI in the oil and gas industry and less on the specific use of ANNs, the present research was proposed to analyze the scientific production of the application of ANNs in this industry in the last five years, using the Scopus database as a reference, to quantitatively analyze the main characteristics of the research published on the subject, in order to evaluate and understand the main trends in the use of ANNs in the oil and gas industry, contributing to the global knowledge on this important subject for the industry.

II. METHODOLOGY

A. Information source

For the development of the bibliometric analysis, the Scopus database was used, which is considered one of the most exhaustive in the field of scientific publication. For this purpose, the official web page of the indexer and the database available for the year 2024 were consulted. For the extraction of the data, the selection criteria were established as articles between 2020 and 2024, as thematic sub-areas: Energy, Engineering, Chemical Engineering, Chemical, Material Science, and Environmental Science. The document type was filtered by Article, Conference Paper, Review, and Conference Review. The type of publication was established as Journal and Proceeding. Since it was impossible to obtain documents written in Spanish, the search was limited to documents in English. The above generated the following equation as a search engine:

(TITLE-ABS-KEY(oil AND gas AND industry AND artificial AND neural AND networks) AND PUBYEAR > 2019 AND PUBYEAR < 2025 AND (LIMIT-TO (SUBJAREA,"ENER") OR LIMIT-TO (SUBJAREA,"ENGI") OR LIMIT-TO (SUBJAREA,"CENG") OR LIMIT-TO (SUBJAREA,"MATE") OR LIMIT-TO (SUBJAREA,"ENVI") OR LIMIT-TO (SUBJAREA, "CHEM")) AND (LIMIT-TO (DOCTYPE,"ar") OR LIMIT-TO (DOCTYPE,"cp") OR LIMIT-TO (DOCTYPE,"cr") OR LIMIT-TO (DOCTYPE,"re") OR LIMIT-TO (DOCTYPE,"ch")) AND (LIMIT-TO (SRCTYPE,"j") OR LIMIT-TO (SRCTYPE,"p")) AND (LIMIT-TO (LANGUAGE,"English")))

A total of 267 documents were obtained that met the selection criteria according to the filtering performed.

B. Indicators extracted

The obtained documents contained relevant information for the bibliometric analysis, such as the country of origin of the research, authors, institutional affiliation, sub-area, year of publication, type of document, keywords used, and the specific process where ANNs were used in the oil and gas industry.

C. Information analysis

The information was analyzed using the analysis tool provided by Scopus to obtain the totals of the indicators and the database downloaded for subsequent descriptive processing using the statistical software JASP v. 0.19.1 and the graphs of results using the office software LibreOffice Calc v. 24.2.6. 24.2.6. For the analysis of co-occurrence of authors, countries, keywords, and affiliations, the bibliometric software VOSviewer was used, which displays the information in maps that were then interpreted according to the objective of the study and the indicators analyzed.

III. RESULTS AND DISCUSSION

A. Documents by publication year

The distribution of the documents retrieved according to the year of publication showed a fairly homogeneous trend (Figure 1), with 2021 being the year in which most research was published with 60, representing 22.5%. In second place, 56 documents were published in 2023, 21.0%. In 2020 and 2022, an equal number of documents were published (52), representing 19.5% in both years and 2024 (47), corresponding to 17.6%.

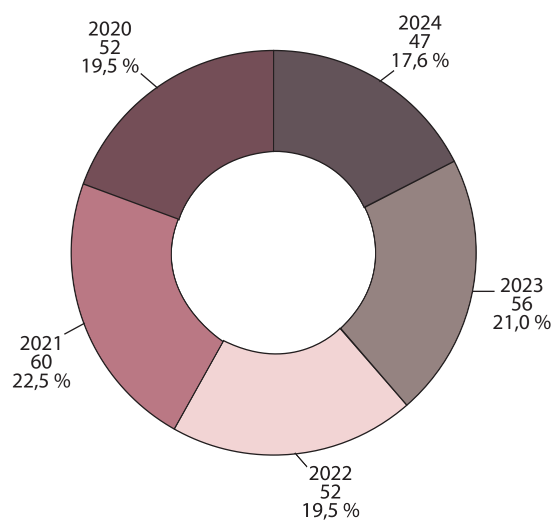

Fig. 1. Distribution of documents published by year.

The growth of AI and its use in industry has evolved in recent years, in the conception of the so-called Industry 4.0, which has created an unprecedented technological revolution in all production processes [21]. Being ANNs one of the most widely used AI tools, it was to be expected a fairly homogeneous document production in the last 5 years, as observed in reviews by different authors in specific areas such as process optimization [22], in solid waste treatment [23], in building construction [24], in refrigeration systems [25], among others. This shows the importance of this topic in recent years and supports the trend observed in the use of ANWR in the oil and gas industry.

B. Documents by publication type

Regarding the type of document published (Figure 2), the largest number were original articles in scientific journals (59.9%), with a significant percentage of articles presented at conferences (35.6%). The minority were review papers published in scientific journals and articles presented at conferences (4.4% between the two).

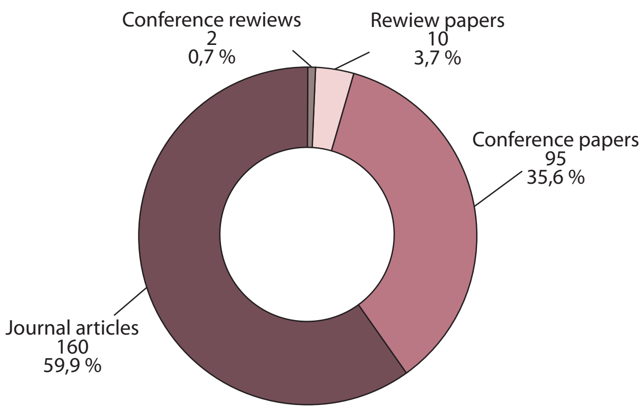

Fig. 2. Distribution of documents published by type.

The publication of research results is a crucial step in scientific development and, in general, the most suitable media for this purpose are scientific journals; therefore, it is to be expected that a majority of the documents retrieved regarding the use of ANNs in the oil and gas industry come from this source. In this regard, the publication of research results in high impact scientific journals is fundamental for the development of engineering and technology, which is in agreement with what has been obtained [26]. On the other hand, the fact that the rise of Information and Communication Technologies (ICT) has been an incentive for the tendency to publish in scientific journals, due to the accessibility that these technologies have given to authors to place their articles, in addition to the access to a greater amount of information [27].

In engineering, scientific congresses have always been taken very seriously as a means for the dissemination of knowledge and research results, in the form of papers and conferences [28]. For this reason, articles published in congresses and conferences tend to be the second most important for the subject studied. Scientific conferences are of utmost importance, not only in the dissemination of information and research results, but also as social events, for the exchange of information and experience directly [29], this makes the results obtained in terms of the number of papers published in conferences justified.

C. Documents by sub-areas

In the analysis of the sub-areas (Figure 3), 69.8% of the documents retrieved correspond to Energy and Engineering (Miscellaneous), with a homogeneous contribution from the other sub-areas taken as filtering parameters. Chemical Engineering was the third most important (9.7%), followed by Environmental Sciences, Chemistry, and Materials Sciences with 7.8%, 6.8%, and 6.0%, respectively.

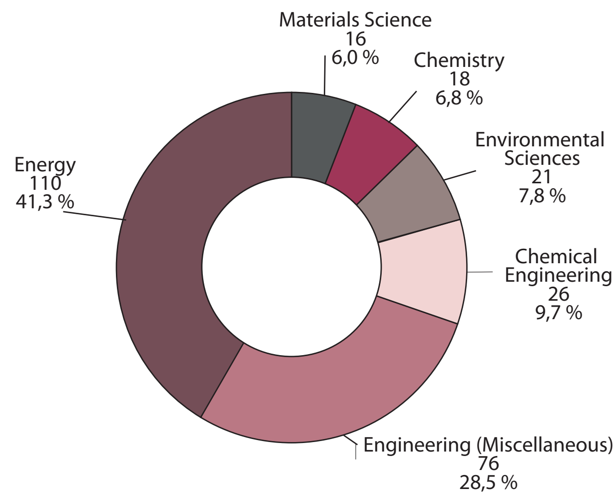

Fig. 3. Distribution of published documents by sub-area.

As the oil and gas industry is the most important industry among those belonging to the energy area, it is logical to observe that this sub-area of research is the one that contributes the largest number of published papers. The oil and gas industry supplies 70% of the world's energy needs [30] so, understandably, publications are preferentially directed towards this area. In this same context, that the oil and gas industry has been influenced by global trends towards renewable and low-carbon energy sources, however, it has been adjusting to changes, especially in terms of technology to adapt to the market, environmental and social trends within the framework of the energy transition, which is not yet fully developed, so oil and gas are still the main energy sources and will be for many years to come [31].

D. Documents by country of origin

The countries with the highest research production for using ANNs in the oil and gas industry are China, the United States of America, Saudi Arabia, Iran, Brazil, India, Canada, Malaysia, Russia, Germany, and Nigeria (Figure 4). These 11 countries account for 61.8% of all published papers. Rounding out the list are another 50 countries accounting for 38.2%. The most productive were China with 39 papers, the United States of America with 35 papers, and Saudi Arabia with 34 papers.

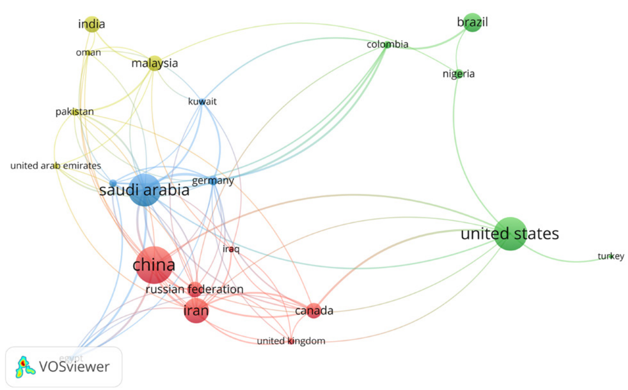

Fig. 4. Map of occurrence of country of origin of the documents.

According to the Scimago Journals & Country Rank, the countries with the highest global scientific production are the United States of America and China, which is consistent with what was obtained and corroborates that these two countries are also the ones with the highest production in the subject under study. In the oil and technology areas, China represents a country with significant progress in recent years, as corroborated by the studies indicating that Chinese research in the oil and gas industry is focused on enhanced oil recovery with the use of state-of-the-art technology and intelligent systems [32], which is consistent with their greater number of papers in the use of ANN. Likewise, it has been noted that China is using AI in all phases of oil exploration and exploitation, so a considerable amount of research where ANNs have been used as AI tools is to be expected [33].

Regarding the United States of America, the use of AI in the oil and gas industry is also widespread with studies deriving from research in areas such as reservoir analysis and especially the prediction of saturation pressures [34]. Although Saudi Arabia is not among the top producers of scientific papers globally, being one of the largest oil producers in the world, a significant share of papers on the subject under study was to be expected. International collaboration in research has led to its development in Saudi Arabia [35], while it is also credited with increasing in production to the effectiveness of government regulations and financial incentive plans to increase the number of articles published in various scientific fields [36], which has led to an increase in scientific production in an area of knowledge as important for this country as the oil industry.

E. Documents by authors

When analyzing the scientific production in the use of ANN in the oil and gas industry according to the main authors (Figure 5), it was observed that the author with the highest number of published papers is Eftekhari-Zadeh, Ehsan with 32, representing 12.0% of the papers, followed by Mayet, Abdulilah Mohammad and Hanus, Robert with 19 papers (7.1%) each, and in third place Salama, Ahmed S. with 12 authorships (4.5%). A total of 1073 authors were counted. In terms of citations, Nazemi, Ehsan with 219, Hanus, Robert with 159, Lui, Wei with 148, and Eftekhari-Zadeh, Ehsan with 122.

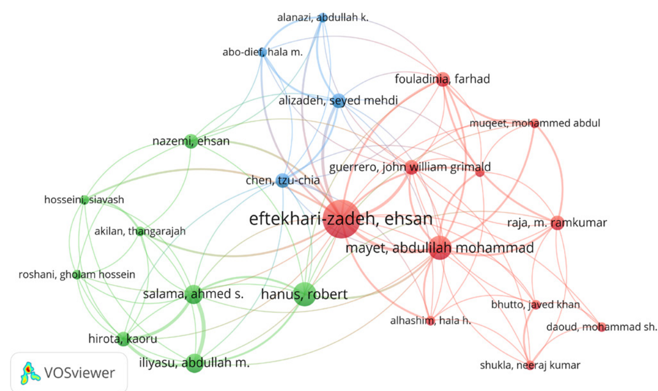

Fig. 5. Map of co-occurrence of authors.

It was observed that the author with the highest number of publications, Eftekhari-Zadeh, Ehsan, is affiliated with the Friedrich Schiller University Jena in Germany, which contributes significantly to the fact that this country is among the most productive in the subject studied. On the other hand, Mayet, Abdulilah Mohammad is a researcher attached to the King Khalid University of Saudi Arabia, and Hanus, Robert belongs to the Rzeszow University of Technology in Poland. From the above, it can be seen that only one of the three major producers of scientific papers related to the use of ANNs in the oil and gas industry belongs to one of the top research producing countries, with a low participation of authors from China and the United States of America, which is not consistent with the record of the top producing countries. From China, Chen, Tzu-Chia is identified with only three papers.

In the case of China, there is a large dispersion of authors with few papers, mostly in projects that were carried out in international collaboration, something that has led to the generation of a large number of scientific papers by this country [37], [38]. This trend seems to favor the number of papers published by the country, but not the amount of individual production, as corroborated in the present research.

F. Documents by affiliation

The institutional affiliation of the documents published on the subject studied was dominated by the King Fahd University of Petroleum and Minerals and the Saudi Arabian Oil Company, both institutions located in Saudi Arabia, with 13 documents, representing 4.9% each (Figure 6). Other institutions appearing among those with the highest number of papers are Universiti Teknologi PETRONAS of Malaysia with 10 papers (3.7%), Friedrich-Schiller-Universität Jena of Germany with 8 papers (3.0%) and Politechnika Rzeszowska im. Ignacego Łukasiewicza of Poland with 7 papers (2.6%). The list is completed by 364 other institutions, where oil companies account for 67.1% of the research on the use of ANNs and the remaining 32.9% corresponds to universities (28.8%), Institutes of Higher Education (3.0%) and Schools of Higher Education (1.1%).

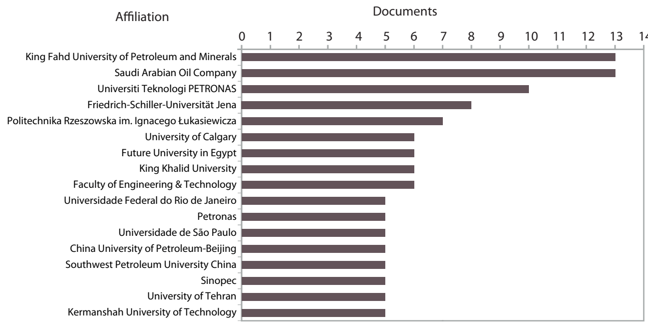

Fig. 6. Affiliations of retrieved documents.

The presence of Saudi Arabian institutions as those with the highest production is due to their dependence on oil exploitation, which has led to the generation of a considerable amount of research in this area, in addition to the use of AI technologies, which leads this industry to focus on its research. This also adds to the increase in research incentives, not only at the governmental level but also at the industrial level, so it can be seen that the first two institutions are a university and an oil company [36].

Again, it is striking that the institutions of the most productive countries (China and the United States of America) do not appear among those with the highest production, where the best placed is China, University of Petroleum-Beijing with 5 documents, and for the United States of America, The University of Texas at Austin with 3 documents. This presents a similar panorama to what happened in the case of the authors.

Due to the importance of the subject matter for the industry and its greater financing power, it can be seen that most of the research is carried out within the industry. Despite this reality, no evidence in previous research corroborates what has been observed, or that has focused on this aspect, which leaves an open gap in this direction. University-industry collaboration has been highlighted, which may explain what has been observed [39], [40], [41], [42]. Since a significant percentage of cases, research carried out within the framework of this collaboration can be found, which leads to significant participation of companies as affiliation in the retrieved documents.

G. Documents by origin

Regarding the origin from which the documents referring to the use of ANNs in the oil and gas industry were extracted, 25 main sources were counted, including scientific journals, congresses, and conferences (Figure 7). In the Journal of Petroleum Science and Engineering, 13 papers were published (4.9%), in Geoenergy Science and Engineering and Society of Petroleum Engineers-SPE Nigeria Annual International Conference, 10 papers were published, that is, 3.7% in each one. Completing the top sources was the journal Energies with 9 papers (3.4%).

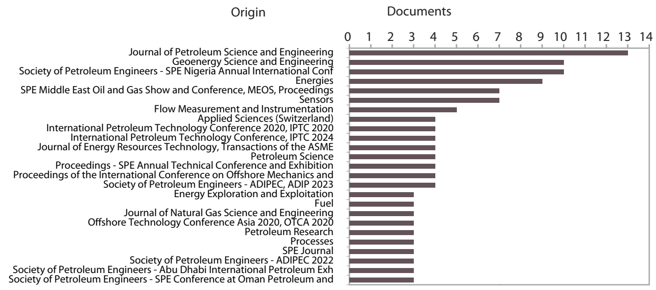

Fig. 7. Origin of retrieved documents.

Scientific journals accounted for 56.0% of the origin of the documents, with the Society of Petroleum Engineers (SPE) conferences responsible for 24.0% of the publications, the remaining 20.0% being obtained from other sources.

The above corroborates what was obtained regarding that most of the documents come from scientific journals, without subtracting the importance of conferences and congresses that represent 44.0% because even though the scientific dissemination media par excellence is the indexed scientific journal, in engineering the presentation of research in congresses and conferences, and its subsequent publication as part of the proceedings of the same, is a common practice that contributes to the dissemination and exchange of knowledge [43], [44], [45].

H. Keyword co-occurrence

The keyword co-occurrence allowed not only to identification of the words and phrases most used in published research on the subject under study but also the processes and operations of the oil and gas industry where ANNs have been applied as a tool for their improvement and optimization. Figure 8 shows the co-occurrence map of the keywords, where it is evident that the most used were Artificial Neural Networks, Machine Learning, Random Forest, and Convolutional Neural Networks.

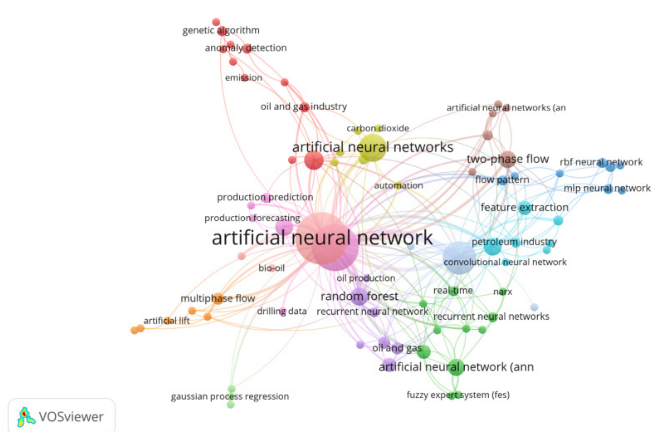

Fig. 8. Keyword co-occurrence distribution map.

Among the processes and operations where ANNs have been used, production operations, multiphase flow, artificial lift, drilling, two-phase flow, extraction, flow patterns, production prediction, emissions, anomaly detection, automation, and carbon dioxide detection were identified.

Reference [9] indicated that ANNs has been applied in all phases of the oil industry (exploration, drilling, production, and reservoir studies) showing reasonable effectiveness, which is consistent with what was obtained in the present bibliometric analysis. Other research also highlighted the use of ANNs in different areas of the oil and gas industry, such as the study of oil production forecast rate through ANNs [46]. ANNs were also applied in well log analysis and demonstrated their flexibility and applicability in contrast to traditional methods [47]. The applicability of ANNs for penetration rate prediction in drilling operations was also highlighted [48].

The results indicate, in the last five years, a trend towards the use of ANNs in traditional areas such as drilling [49], [50], [51] and oil and gas production [52], [53], [54]. However, it has diversified its use in other areas such as pollutant gas emissions [55], [56], corrosion [57], [58], and flow patterns [59]. This trend of the oil industry to apply AI tools such as ANNs in all its processes and to diversify their use is consistent with previous research where it has been noted that, AI tools are driving the optimization of industrial processes and driving innovation in different areas of the industries [60]. Has also demonstrated the applicability of ANNs in the prediction of the corrosive tendency of natural gas [5], which is consistent with the trend observed in this area of knowledge.

V. CONCLUSION

The scientific output on the use of ANNs in the oil and gas industry has been relatively stable in terms of papers published per year, ranging from 47 papers (2024) to 60 papers (2021). This is evidence that the research and production of scientific papers on the subject during the period under study shows an importance that is maintained over time, and demonstrates the importance given to ANNs in the oil and gas field worldwide.

Even though scientific journals continue to be the ideal media for the dissemination of research results, it was found that presentations at indexed congresses and conferences represent an important percentage in the publication of full-text scientific papers, which shows the relevance that engineers and oil companies give to these events for the dissemination of knowledge.

In terms of knowledge sub-areas, the papers published in Energy and Engineering stood out, with a minority participation from other fields such as Chemical Engineering, Environmental Sciences, Chemistry and Materials Sciences. This suggests that research has been generated mainly from the perspective of researchers associated with the oil and gas industry, with topics focused on energy efficiency and improving engineering operations.

The countries with the highest oil production are the ones that are generating the greatest amount of research in the use of ANNs, due to the importance they give to innovation in their operations and process optimization, which also leads to a significant participation of industries as producers of scientific documents, displacing universities in their role of knowledge production and research.

Researchers from Arab and Asian countries have devoted the most effort to studying the applicability of ANNs in oil and gas operations. This is evidenced by the greater number of authors from countries in these two regions, with the most prolific author being Ehsan Eftekhari-Zadeh, who produced 12.0% of the papers.

The King Fahd University of Petroleum and Minerals and the Saudi Arabian Oil Company, both institutions located in Saudi Arabia with 13 documents each, were the institutions with the highest number of appearances as institutional affiliations of the authors. This shows the importance given to the study of the use of NAR in oil and gas operations in Saudi Arabia as an oil producing country. Other institutions that appear as important generators of documents on the subject analyzed were the Universiti Teknologi PETRONAS of Malaysia, Friedrich-Schiller-Universität Jena of Germany and Politechnika Rzeszowska im. Ignacego Łukasiewicza from Poland, which shows that this subject is not only developed in Arab countries, but there is also a significant production in Europe.

Most of the papers were published in scientific journals, the most important being the Journal of Petroleum Science and Engineering. There were also publications in conferences, especially those of the Society of Petroleum Engineers (SPE). The results indicate that scientific journals in the field of petroleum science and engineering are considered to be the ideal media for the diffusion of research on the subject studied, but importance was also given to SPE conferences as a means of diffusion due to the relevance of this organization in the world petroleum field.

According to the keyword co-occurrence analysis, the use of ANNs in the oil and gas industry has focused on basic exploration, production and reservoir operations; however, there is a trend toward other areas that affect the petroleum system, such as the study of flow patterns, the prediction of pollutant emissions to the environment, especially carbon dioxide, the detection of operational problems, corrosion and the automation of operations.

Given that the bibliometric analysis was limited to the last five years and only to documents published in Scopus, it is recommended to extend the study period and use other databases such as SciELO or DOAJ where documents published in Spanish can be found, which can generate a broader panorama of scientific production in this area, especially by including research by Latin American authors from oil and gas producing countries.

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Monitoring the removal of a mixture of emerging pharmaceutical contaminants assisted by a fixed TiO_2 support in a photocatalytic process

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***Abstract* — This study evaluated the efficacy of removing estradiol, sulfamethoxazole, and paracetamol from water using titanium dioxide (TiO_2). A layer of TiO_2 was fixed onto ceramic tiles and exposed to a solution of the pharmaceuticals under 254 nm ultraviolet light. The TiO_2 exhibited a surface area of 2.78 m^2/g with Methylene Blue, which favors the adsorption and subsequent degradation of the pharmaceuticals. After 60 minutes of exposure, the removal of estradiol was 69.43%, paracetamol 50.84%, and sulfamethoxazole 24.80%. Additionally, it was determined that the degradation kinetics of each drug varied, with some fitting first-order models (estradiol and paracetamol) and others fitting second-order models (sulfamethoxazole). The time in minutes required for the drug concentration to decrease to one-tenth of its original concentration was 107 for estradiol, 190 minutes for paracetamol, and 244 for sulfamethoxazole. Photocatalysis with TiO_2 immobilized on ceramics can be used to treat water contaminated with mixtures of pharmaceuticals without observing a restrictive effect between the drugs.**

***Keywords:* photocatalysis; Titanium dioxide; emerging pharmaceutical contaminants.**

***Resumen* — Este estudio evaluó la eficacia de la remoción de estradiol, sulfametoxazol y paracetamol del agua utilizando dióxido de titanio (TiO_2). Para ello se fijó una capa de TiO_2 sobre baldosas cerámicas y se expuso a una solución de los fármacos bajo luz ultravioleta de 254 nm. El TiO2 presentó un área superficial de 2.78 m^2/g con Azul de Metileno lo que favorece a la adsorción y posterior degradación de los fármacos. La foto remoción después de 60 minutos de exposición del estradiol fue del 69.43%, del paracetamol 50.84% y del sulfametaxazol 24.80%. Además, se determinó que la cinética de degradación de cada fármaco variaba, ajustándose algunos a modelos de primer orden (estradiol y paracetamol) y otro a segundo orden (sulfametaxazol). El tiempo en minutos necesario para bajar al 10% la concentración original de los fármacos fue de 107 para el estradiol, 190 minutos para el paracetamol y 244 para el sulfametaxazol. La fotocatálisis con TiO_2 inmobilizado en cerámicas puede ser utilizada para el tratamiento de aguas contaminadas con mezclas de fármacos sin que se observe un efecto restrictivo entre los fármacos.**

***Palabras Clave:* fotocatálisis; Titanium dioxide; emerging pharmaceutical contaminants.**

I. INTRODUCTION

THE presence of pharmaceuticals in wastewater can cause toxicity in aquatic organisms due to their ability to bioaccumulate and the adverse effects they can produce. The bioaccumulation capacity of these compounds can be manifested in the food chain, resulting in dangerous concentrations of pharmaceuticals in food due to biomagnification, affecting not only aquatic organisms but also predators, including humans [1], [2], [3]. Among the different pharmaceuticals, those of greatest interest due to the associated risks are endocrine disruptors and antibiotics.

Continuous exposure to low concentrations of pharmaceuticals or other endocrine disruptors through the consumption of contaminated water or aquatic products can have long-term effects on human health, such as alterations to the endocrine system and other hormonal problems. One compound that acts as an endocrine disruptor and is present in various pharmaceuticals is estradiol. Estradiol is a steroid hormone that, as an endocrine disruptor, can interfere with the hormonal systems of aquatic organisms, causing effects such as feminization of males, reduced fertility, and alterations in reproductive behaviors. Additionally, estradiol is persistent in the environment and can bioaccumulate, leading to higher concentrations in the food chain and eventually affecting humans, increasing the risk of hormone-dependent cancers and other health problems. Evaluating the presence of estradiol in wastewater is necessary to make decisions to mitigate risks to ecosystems and public health, since exposure through contaminated drinking water can have negative effects, especially in vulnerable populations [4], [5], [6].

The presence of antibiotics can contribute to the development and spread of antibiotic-resistant bacteria, complicating the treatment of infections and representing a serious public

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health problem. One of the most commonly used antibiotics is sulfamethoxazole, often used in combination with trimethoprim, and has a wide range of applications for different types of infections [7], [8]. This compound is resistant to degradation in conventional wastewater treatment plants, allowing its release into the aquatic environment. The presence of sulfamethoxazole in water can cause toxicity in aquatic organisms, including sublethal effects on the growth and reproduction of fish, invertebrates, and algae. Additionally, the bioaccumulation of this antibiotic can lead to harmful concentrations in the food chain, affecting top predators, including humans. The continuous presence of this compound in the environment can contribute to the proliferation of resistant bacteria [9], [10].

Another emerging contaminant of concern is paracetamol, a widely used analgesic and antipyretic, being one of the most used worldwide. Conventional wastewater treatment systems do not always completely remove paracetamol, allowing its release into surface waters. Although paracetamol can degrade relatively quickly under aerobic conditions, it can persist in the environment and its degradation byproducts can be toxic to aquatic organisms [11], [12], [13].

Therefore, it is important to remove these compounds from water. For their treatment, the mechanisms must be considered, as some pharmaceuticals can generate toxic metabolites during their degradation, further complicating the remediation of contaminated waters [14]. Photocatalysis over titanium dioxide (TiO_2) is a technique that has been widely investigated in recent decades due to its effectiveness in the degradation of organic compounds, which can include pharmaceuticals. Studies have shown that photocatalysis can efficiently decompose pharmaceuticals such as ciprofloxacin, sulfamethoxazole, and tetracycline, which are resistant to degradation in conventional wastewater treatment plants. Additionally, photocatalysis has shown effectiveness in the removal of other common pharmaceutical compounds, such as paracetamol and ibuprofen, as well as in the degradation of endocrine disruptors such as bisphenol A and nonylphenol, which can cause adverse effects on health and the environment [15], [16], [17].

This technique is generally carried out in aqueous suspensions of TiO_2, with the most efficient form being the use of titanium dioxide in the form of nanoparticles [18], [19]. The photocatalysis mechanism can be seen in Fig. 1, and is based on the stimulation or excitation of the TiO_2 semiconductor by UV or visible light, whether of natural or artificial origin. The process begins when TiO_2 absorbs photons with energy equal to or greater than its bandgap (3.2 eV for anatase, 3.0 eV for rutile, and 2.8 eV for brookite); this absorption promotes an electron from the valence band to the conduction band, creating an electron-hole pair (e-/h+). These pairs in the catalyst participate in redox reactions, see Figure 1. The holes (h^+) can oxidize water molecules or hydroxyl ions to form hydroxyl radicals ($^{\bullet}OH$), which are highly reactive species and capable of oxidizing organic contaminants to their complete mineralization, i.e., converting them to CO_2 and H_2O, see Eq. 1 and Eq. 2.

$$h^+ + H_2O \rightarrow \cdot OH + H^+ \tag{1}$$

$$h^+ + OH^- \rightarrow \cdot OH \tag{2}$$

On the other hand, electrons (e-) can reduce dissolved oxygen in water to form superoxide radicals ($O_2^{\cdot-}$) which also participate in the degradation of contaminants [20]. This can be seen in equations Eq. 3, Eq. 4 and Eq. 5

$$e^- + O_2 \rightarrow O_2{\cdot}^- \tag{3}$$

$$O_2{\cdot}^- + H^+ + \rightarrow HO_2 \cdot \tag{4}$$

$$2HO_2 \cdot \rightarrow H_2O_2 + O_2 \tag{5}$$

In most TiO_2 catalyzed photocatalytic studies, the focus has been on determining the optimal operating conditions to achieve the best performance in terms of degradation and mineralization [8], [21]. The operational parameters frequently investigated include photocatalyst loading, initial concentration of the pharmaceutical under investigation, type of photocatalyst, pH of the solution, wavelength, and light intensity [22], [23], [24].

One of the main drawbacks is the difficulty in recovering the catalyst; however, there is little information on studies to immobilize the catalyst and determine its effectiveness. Titanium dioxide can be anchored to a glass or ceramic surface to increase its stability and durability, which promotes a uniform distribution of TiO_2 particles, increasing the stability of the catalyst and allowing it to be reused several times without significant loss of catalytic activity. The ability to fix TiO_2 allows for the optimization of its surface area, which favors greater photocatalytic activity and also reduces secondary contamination that may occur due to the presence of free TiO_2 nanoparticles, which in some cases can have undesirable effects on the environment and human health. Surfaces with anchored TiO_2 can be used to purify water and air, especially organic contaminants, emerging contaminants, volatile organic compounds (VOCs), bacteria, and other toxic substances that may be present in these media. Based on this evidence, so-called self-cleaning surfaces have been developed, which, when exposed to light, can degrade organic contaminants and microorganisms [25].

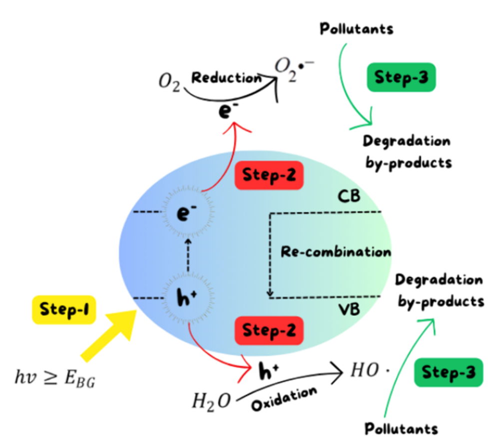

Fig. 1. Photocatalytic process the formation of photoinduced charge carriers (e^-/h^+) on the surfaces of semiconductor particles of TiO_2.

TiO_2-based photocatalytic processes have proven to be highly effective, making it necessary to leverage this knowledge to easily implement and low-cost methodologies to address the growing problem of pharmaceutical residues in small and medium-sized cities. The objective of this work was to evaluate the photodegradation of estradiol, sulfamethoxazole, and paracetamol on a TiO_2-coated glazed ceramic surface as a tertiary wastewater treatment that could be used in small cities or for the treatment of hospital wastewater.

II. MATERIALS AND METHODS

A. TiO_2 Photocatalytic Treatment System

White commercial tiles with a glazed surface were used. A uniform layer of TiO_2 (rutile) paste was spread over these tiles, followed by calcination (900 °C for 4 hours) to ensure proper fixation of the TiO_2 on the substrate. Food-grade TiO_2 (rutile) (supplier: Freire Mejía) was used because it is the most commonly available form and is cost-effective ($TiO_2 \geq 94\%$, rutile $\geq 98\%$, particle size ≥ 45 µm, max. 0.05%). A 23 W UV lamp emitting 254 nm light served as the radiation source. The distance between the radiation source and the reaction surface was set at 20 cm, as shown in Figure 2, which displays the experimental setup.

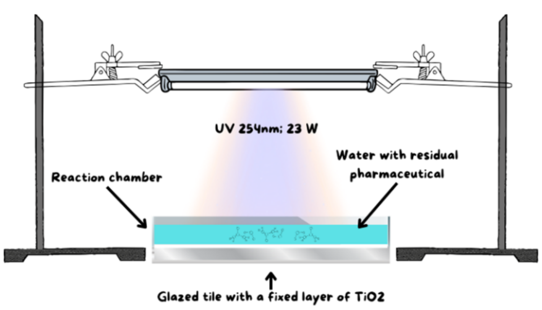

Fig. 2. Representation of the apparatus used for photodegradation

B. Removal tests

An aqueous solution was prepared, consisting of a mixture of three pharmaceuticals at different concentrations: 500 ppb estradiol (Sigma Aldrich), 10 ppm sulfamethoxazole (Sigma Aldrich), and 10 ppm acetaminophen (Sigma Aldrich). For the assay, 50 mL of the solution was placed and exposed to 254 nm UV radiation in the setup shown in Figure 2. Every 10 minutes, 0.5 mL samples were taken for a total of 80 minutes. The treated samples were analyzed by high-performance liquid chromatography (HPLC). The equipment used was an HPLC (Thermo Ultimate 3000) equipped with a 20 cm C18 column, with a detector set at 254 nm for estradiol and 272 nm for sulfamethoxazole and acetaminophen. The mobile phase was a mixture of water (53%), methanol (24%, Fisher chemical, ACS), and acetonitrile (23%, Supelco-LiChrosolv) of HPLC grade. Isocratic conditions were employed, and the column temperature was maintained at 25 °C with a flow rate of 0.9 mL/min. Removal was determined using Eq. 6, where C_{A0} is the initial concentration of the contaminant and C_A is the concentration at time t.

$$\%R = \frac{C_{A0} - C_A}{C_{A0}} \times 100 \tag{6}$$

B. Methodology for determining the surface area of Methylene Blue and BET

The adsorption area of titanium dioxide (TiO_2) was determined using a 5.155 ppm solution of Methylene Blue (MB) dissolved in deionized water. The adsorption process was carried out in a batch system with varying amounts of TiO_2. Subsequently, the concentration of unadsorbed methylene blue was quantified using UV-Vis spectrophotometry at a wavelength of 660 nm, employing a Thermo Scientific Evolution 60 UV-Vis spectrophotometer.

The surface area was determined by N_2 adsorption using the Brunauer, Emmett, and Teller (BET) theory at 77.6 K using a Micromeritics Autochem 2920 instrument. Each sample was degassed at 373 K for 720 minutes under a vacuum of 10^{-4} Pa.

C. TiO_2 Photocatalytic Treatment System

The kinetic calculations were performed using the Langmuir-Hinshelwood (L-H) kinetic model. This model assumes that the rate-determining step (RDS) of the photocatalytic reaction involves the presence of the reactant as a monolayer at the photocatalyst/solution interface. The Eq. 7 for this model is:

$$r_0 = \frac{(k_C K[C_0])}{(1 + K[C_0])} = k_{obs}[C_0]^n \tag{7}$$

Where:

r0 is the initial rate of photo-oxidation of the solute.
kc is the rate constant of the photo-oxidation ste==p.
K is the stability constant of the drug-TiO_2 equilibrium.
n is the order of the kinetics.

For n=0, the kinetics follow a zero-order rate law, and the Langmuir-Hinshelwood (L-H) model simplifies to a simpler expression (Eq. 8).

$$r_0 = k_{obs} \tag{8}$$

In this work, both constants (kc and K) were obtained by regression analysis of initial rates and corresponding initial drug concentrations. Calculations were performed using the Solver add-in in Microsoft Excel.

III. RESULTS AND DISCUSSION

A. Measurement of the specific surface area of TiO_2

The experimental data for the adsorption isotherm calculations are summarized in Table 1. Co represents the initial Methylene Blue concentration, Ce the equilibrium concentration, and qe the amount adsorbed per unit mass of TiO_2. Methylene blue (MB)

($C_{16}H_{18}ClN_3S$) is an organic compound widely used in the determination of the specific surface area of clays, activated carbon, and other types of adsorbents. In solution, this dye ionizes, forming a cation that is electrostatically attracted to negatively charged surfaces. By measuring the amount of MB adsorbed, it is possible to calculate the total exposed area of the adsorbent particles. The adsorption of MB onto titanium dioxide (TiO_2) fits the Langmuir isotherm model, characteristic of a monolayer coverage [26]. The Langmuir nature of the adsorption process is evident from the isotherm plot in Figure 3.

TABLE I
VALUES FOR THE METHYLENE BLUE ADSORPTION ISOTHERM CALCULATIONS ON TIO_2

Masa TiO_2 (g)	Co mg/L	Ce mg/L	qe mg/mg
0.0095	5.155	3.052	0.0221
0.0439	5.155	2.191	0.0067
0.1408	5.155	1.518	0.0025
0.6124	5.155	0.160	0.0008

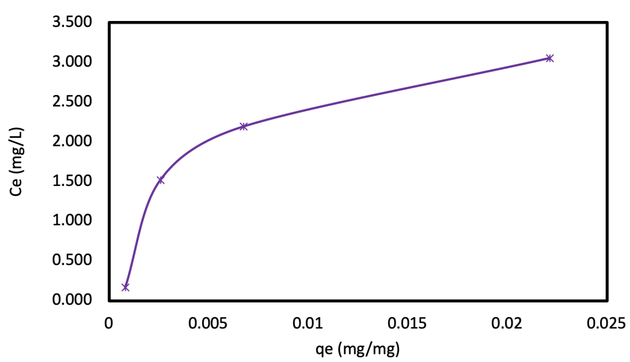

Fig. 3. Methylene Blue adsorption isotherm on TiO_2

From the Langmuir isotherm results, it was determined that the TiO_2 used had a surface area of 2.78 m²/mg, as measured by Methylene Blue.

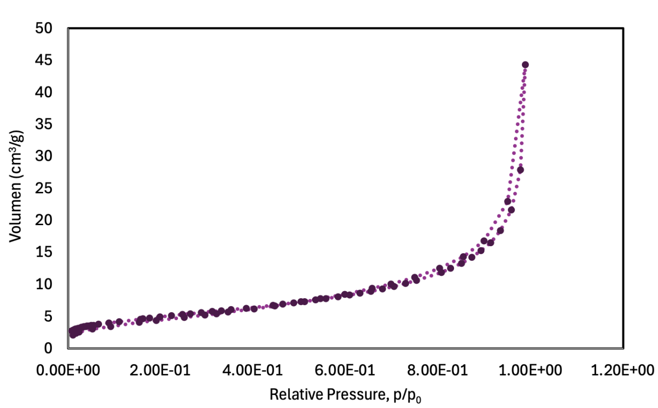

Fig. 4. BET isotherm with N_2 of TiO_2

Figure 4 shows a typical type IV isotherm characteristic of mesoporous solids. A pore volume of 0.033 cm³/g, a 12 m²/g surface area, and a measured pore width of 14.48 nm were obtained.

The N_2 BET isotherm (Figure 4) results of the TiO_2 correspond to a type IV curve characteristic of mesoporous materials, indicating the presence of intermediate-sized pores with a hysteresis H4. The pore volume of 0.033 cm³/g suggests moderate porosity, confirming the highly porous nature of TiO_2. The average pore width of 14.48 nm indicates that these pores are large enough to allow the diffusion of considerably sized molecules. These values characterize TiO_2 as a mesoporous solid with high adsorption capacity and excellent catalytic activity.

The surface area results obtained by the BET method, and the surface area measured by the MB method show a high correlation. It is important to consider that the MB method, based on the adsorption of large molecules such as methylene blue, may underestimate the total surface area, especially in microporous materials, due to the limitations of access of these molecules to the smallest pores. In this case, the correlation between both methods suggests that most of the accessible surface area is composed of mesopores, large enough to allow the adsorption of methylene blue molecules. This characteristic is of great relevance for applications involving the adsorption of considerably sized organic molecules, since the extensive mesoporous surface provides numerous accessible adsorption sites for these molecules [27].

B. Removal of pharmaceuticals

The concentration of the pharmaceuticals used in the mixture was measured using HPLC. The results of the chromatograms obtained from the measurements over time have been compiled and are presented in Figure 5.

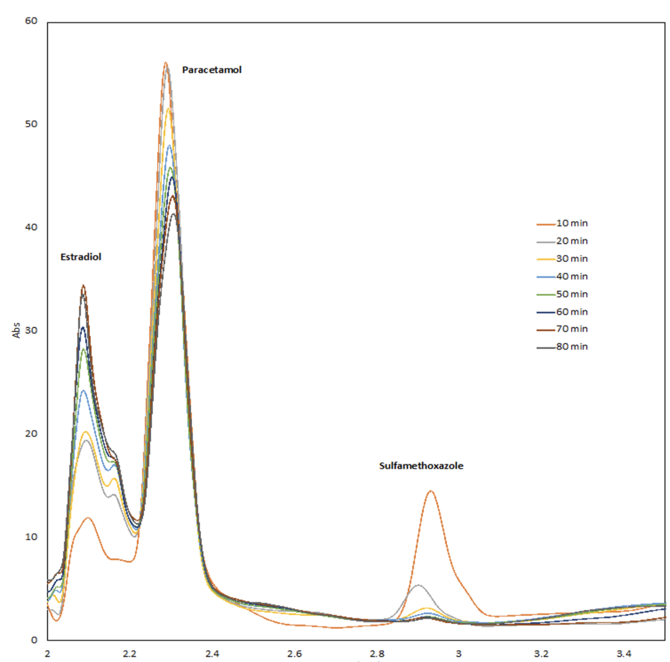

Fig. 5. Drug degradation measurement chromatograms

Figure 5 shows a change in the analyte concentration over time due to exposure to 254 nm UV radiation. The results of applying the integral method to the concentrations are shown in Figure 6. Estradiol (k = 0.0218 1/min) and paracetamol (k = 0.046 1/min) showed a better fit to the first-order model, while sulfamethoxazole (k = 0.048 L/mg min) fit a second-order kinetic model.

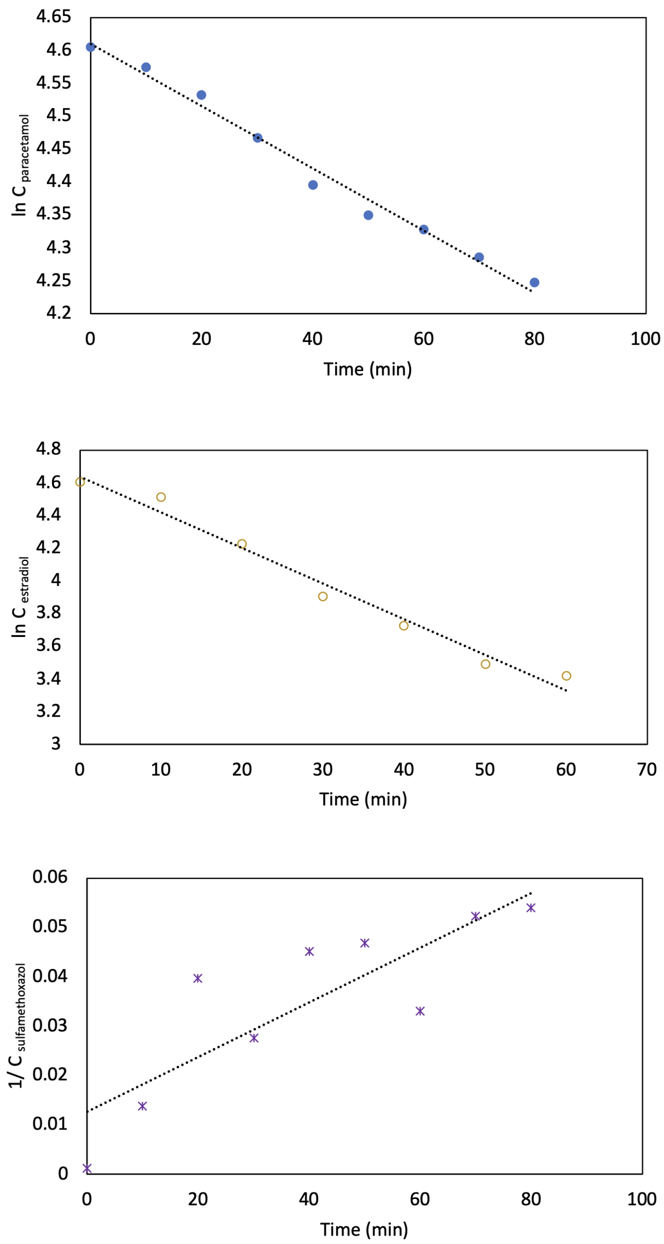

Fig. 6. The concentration changes of the pharmaceuticals due to the removal process and the relationship needed to determine their kinetic type: (a) Estradiol fitted to the first-order integral model; (b) Paracetamol fit to the first-order model; (c) Sulfamethoxazole fitted to a second-order integral kinetic model.

The rate constants, kc and K, for the photo-oxidation reactions were obtained by non-linear GRG optimization using Solver. The optimized values, subject to the constraints of positive kc and K > 1, are summarized in Table 2.

TABLE II
K AND KC RATE CONSTANTS OF THE PHOTO-OXIDATION EQUATION AND TIME TO REDUCE DRUG CONCENTRATION TO ONE-TENTH OF ITS INITIAL VALUE

Pharmaceuticals	K (L/mg)	kc (mg/L min)	t (c/10 min)
Estradiol	4.13	0.056	107
Paracetamol	1.15	0.97	190
Sulfametoxazol	1.2	0.010	244

The results demonstrate a clear correlation between the reaction rate constant (kc) and the time required to reduce drug concentration by 90% (t(C/10)). Higher kc values indicate faster degradation rates. Pharmaceuticals adsorbed on TiO_2 are expected to be more mobile, enhancing their interaction with hydroxyl radicals. This mobility can be influenced by drug chemistry, drug-surface interactions, and TiO_2 surface roughness [28].

The experimental data obtained corroborate the efficacy of the proposed method for the degradation of the studied pharmaceuticals. The observed reduction percentages after 60 minutes of irradiation are significant, especially in the case of estradiol (69.43%), although for the other pharmaceuticals the removal was also significant, with paracetamol (50.84%) and sulfamethoxazole (24.80%), indicating a high potential of this technology for the treatment of wastewater contaminated with pharmaceutical compounds [29]. However, it is important to note that the efficiency of degradation can vary depending on various factors, such as the initial concentration of the pharmaceuticals, the intensity of the radiation, and the presence of other compounds in the water. To optimize photocatalytic processes and expand their application to a variety of contaminants, more detailed studies are needed on the reaction mechanisms, the influence of operational variables, and the combination of photocatalysis with other treatments [28].

IV. CONCLUSIONS

The kinetic constant values presented in Table 2 offer a simplified view of the photo-oxidation of a drug mixture. The Langmuir-Hinshelwood model used, while useful for understanding fundamental processes, does not capture the complexity of real systems, where the presence of multiple compounds and the formation of degradation products can significantly alter the reaction kinetics. Although the obtained results provide an initial estimate of degradation rates, it is essential to recognize that to accurately describe these systems and optimize wastewater treatment processes, more sophisticated kinetic models are required that incorporate the dynamics of competitive adsorption and the formation of reaction products.

The degradation percentages obtained in this study are consistent with the results reported in previous research on heterogeneous photocatalysis using titanium dioxide under various experimental conditions [11], [17], [29]. This consistency suggests that the proposed method, based on the application of a titanium dioxide layer and exposure to UV radiation, demonstrates considerable robustness. Unlike other approaches that require complex operating conditions, the system allows for significant degradation levels to be achieved with a simplified configuration. This simplification reduces implementation complexity and cost, facilitating its application in diverse environments. The viability of a system that relies on accessible factors such as UV light and a basic catalytic surface opens new possibilities for decentralized wastewater treatment. The ability to obtain results comparable to other methods, without relying on additional reagents, underscores the potential of this technology as a practical and economical solution to address water contamination at various scales

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Human resources - a critical success factor for quality and sustainability in the industry

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Abstract — **Quality (QUA) in industry encompasses several critical success factors (CSF), including human resources (HR), and the production process is of paramount importance; consequently, quantifying their impact and contribution is essential for sustainability. This study presents a structural equation model (SEM) that relates managerial commitment (MAC) as an independent variable, operators (OPE), suppliers (SUP), and lean manufacturing tools (LMT) as mediating variables, and QUA as a sustainable response variable. The variables were interconnected through six hypotheses, each validated using data from 286 responses to a questionnaire administered to the Mexican maquiladora industry. The SEM was validated using the partial least squares (PLS) approach, and a sensitivity analysis was also performed. The findings indicate that MAC has direct and positive effects on OPE, LMT, and SUP, with the former exhibiting the strongest influence. Similarly, OPE, LMT, and SUP directly affect QUA for sustainability, with the latter demonstrating the most significant impact. The study concludes, statistically and empirically demonstrates that human factors (managers, SUP, and OPE) and production systems can ensure product QUA and economic sustainability, thereby reducing defects and customer returns.**

Keywords: **management commitment; Operators; Suppliers; QUA; Sustainability.**

Resumen — **La calidad (QUA) en la industria abarca varios factores críticos de éxito (CSF), incluidos los recursos humanos (RR. HH.), y el proceso de producción es de suma importancia; en consecuencia, cuantificar su impacto y contribución es esencial para la sostenibilidad. Este estudio presenta un modelo de ecuaciones estructurales (SEM) que relaciona el compromiso directivo (MAC) como variable independiente, los operadores (OPE), los proveedores (SUP) y las herramientas de fabricación ajustada (LMT) como variables mediadoras, y la QUA como variable de respuesta sostenible. Las variables se interconectaron a través de seis hipótesis, cada una validada utilizando datos de 286 respuestas a un cuestionario administrado a la industria maquiladora mexicana. El SEM se validó utilizando el enfoque de mínimos cuadrados parciales (PLS), y también se realizó un análisis de sensibilidad. Los resultados indican que MAC tiene efectos directos y positivos en OPE, LMT y SUP, siendo el primero el que ejerce una mayor influencia. Del mismo modo, OPE, LMT y SUP afectan directamente a QUA en cuanto a sostenibilidad, siendo este último el que demuestra el impacto más significativo. El estudio concluye, demostrando estadística y empíricamente, que los factores humanos (directivos, SUP y OPE) y los sistemas de producción pueden garantizar la sostenibilidad económica y de QUA de los productos, reduciendo así los defectos y las devoluciones de los clientes.**

Palabras Clave: **Compromiso de la dirección; Operadores; Proveedores; Calidad; Sostenibilidad.**

I. INTRODUCTION

QUALITY (QUA) is a complex concept that refers to the degree to which a product meets predefined characteristics and satisfies customer needs and expectations; however, human resources (HRs) are responsible for this [1]. This QUA depends on several factors such as the high management commitment (MAC), operators (OPE), and suppliers (SUP) of raw materials, all of which refer to people.

High product QUA enhances organizational competitiveness, sustainability, and customer satisfaction, resulting in increased sales and loyalty. Furthermore, they contribute to the reduction of waste and resource utilization [2]. Human resource departments play a critical role in achieving QUA assurance standards through planning, coordinating, and supervising activities. They have developed and implemented policies that align with daily operations and sustainability objectives. Effective communication with OPE facilitates the conveyance of QUA assurance objectives and sustainable procedures while obtaining feedback on challenges and opportunities [3]. Nevertheless, continuous training is essential for OPE to maintain high-QUA assurance standards, necessitating management-authorized resources.

Managers play a crucial role in implementing QUA best practices in production lines, approving economic improvements and investments, adhering to ISO 9001 standards, and establishing sustainable metrics and continuous monitoring programs to identify defects and reduce costs using lean manufacturing (LM). Research indicates that promoting production process improvements enhances product QUA and increases

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job satisfaction. Furthermore, standardized processes using QUA culture are essential [4].

Another HR with which managers interact outside the company is SUP. These managers are responsible for integrating SUP and their incorporation into the production process, as they possess knowledge of the technical characteristics of the supplied raw materials and can propose improvements to the system and its operations [5]. The extant literature suggests that the effective integration of SUP results in reduced cycle times, optimized inventories, and shared QUA standards, benefiting both customers and manufacturers.

SUP reduce defects in raw materials by offering QUA and participating in manufacturing innovations for sustainable products. They are required to provide technology for new products [6]. Long-term relationships with SUP, characterized by high trust, enable the negotiation of prices and delivery dates, cost reduction, and economic sustainability.

Managers must align OPE, lean manufacturing techniques, and supplier entities to offer QUA and sustainable agreements with human resources, production processes, SUP, production systems, and OPE as critical success factors [7]. However, those who control or manage these entities are managers; thus, MAC is a critical factor upon which many others depend on their decision-making power and access to resources.

Numerous studies have analyzed the critical success factors for QUA. For instance, Fotopoulos and Psomas [8] related the critical factors of Total QUA Management to the organizational and economic performance of companies, and Carmona-Márquez, *et al.* [9] analyzed whether all factors that favor QUA success have the same impact, and determined that human resources excel over others by being the executors of production plans and programs. Bubb [10] asserted that human resources must be reliable and skilled in generating QUA; otherwise, they will make numerous mistakes, resulting in costly defects. Kujawińska, *et al.* [11] indicated that OPE should be motivated by the management to inspect their processes and machines. Fu, *et al.* [12] argue that SUP are also the basis of QUA for manufacturers. Khalili, *et al.* [13] reported that QUA is achieved in the production process with the support of the OPE and SUP. However, these studies analyze human factors and the productive process in isolation as critical success factors of QUA, and do not allow for an integrated analysis linking them. Furthermore, it is not known what occurs if there are low or high levels of implementation for some of these variables, which is limited to speculations without a statistical basis.

This study aims to analyze the human resources involved in generating product QUA (MAC, OPE, and SUP) and the production process and quantify their relationship and impact on the achievement of QUA. It is hypothesized that the independent variable is the MAC associated with managers, who, owing to their decision-making power and access to resources, favor the performance of the OPE, integrate the SUP, and decide which lean manufacturing techniques to integrate into the production process, which are mediating variables that favor product QUA as the dependent variable, a sustainable measurement.

The results of this study will allow managers to have an empirical and statistically validated basis on which to determine the variables that are important to achieve QUA in their products, and thus make better-informed decisions and allocate resources appropriately. To the best of our knowledge, this is the first study to report a probability-based sensitivity analysis to identify the risks of low-level implementation of the latent variables analyzed.

Following this introduction, section two presents a literature review and hypotheses, section three presents the methodology, section four reports the results and discussion, and section five presents the conclusions.

II. LITERATURE REVIEW AND HYPOTHESES

MAC is critical for ensuring QUA, because it directly influences SUP, OPE, and the production process. MAC establishes the foundation for an organization's culture and operating practices, thereby affecting employee motivation, commitment, and sustainability. Literature indicates that managers' strong leadership and commitment to QUA are essential for fostering a productive process that generates QUA. When demonstrated, this instills a sense of purpose and responsibility among employees–a principle of social sustainability.

Achieving QUA standards is not a straightforward process, and OPE' participation in production processes is necessary, with managers responsible for their integration. For instance, involving workers in decision-making enhances their sense of ownership and accountability for QUA outcomes, as they perceive their contributions as valuable and contributory to the product's QUA, subsequently increasing their motivation and morale [14].

Furthermore, MAC with QUA is manifested in the establishment of robust protocols that ensure safety and guide employees in their daily tasks within the production process, emphasizing QUA [15]. Effective QUA management systems in the manufacturing and service industries have been demonstrated to facilitate the organization of operations, define responsibilities, and document processes, which are crucial for maintaining consistent and certifying QUA. Additionally, committed managers consistently allocate the resources necessary to improve production processes, including budgets, personnel, and equipment, to QUA initiatives.

Similarly, MAC ensures the integration of QUA into an organization's strategy. To achieve this goal, managers must select appropriate machines or production methodologies to be implemented in the production system. For example, they are responsible for implementing other LM tools and providing resources such as total productive maintenance (TPM) and quick changeovers (SMED). In conclusion, managers are responsible for continuous improvements in the production process, and those collaborating with OPE can swiftly identify areas of opportunity.

Managers are also responsible for directly liaising with SUP to ensure product QUA [16]. To accomplish this, they must clearly articulate the raw material expectations of SUP, test procedures, and delivery standards, specifying quantities and delivery times. However, they are also responsible for performing tasks that facilitate joint development with SUP, thereby enabling them to improve their processes and maintain a sustainable production line. This typically involves audits, training in the manufacturer's production process, technical assistance, and certification programs, which indicate the level of collaboration.

Consequently, MAC is related to several entities within and outside the company, and the following hypotheses are proposed:

H_1. Management commitment has a direct and positive effect on operators to ensure QUA.

H_2. Management commitment directly and positively affects the Lean manufacturing tools to ensure QUA.

H_3. Management commitment has a direct and positive effect on SUP in ensuring QUA.

However, it is essential to ascertain the direct effects of these variables (SUP, OPE, and LMT) on product QUA in a direct manner. For instance, Febriani, *et al.* [17] determined that OPE significantly influence product QUA through decision-making and adherence to QUA control protocols in production lines. They can prioritize activities and processes that facilitate compliance with time, quantity, and established standards [18]. Furthermore, OPE are the primary identifiers of defects when performing self-inspection, and they require knowledge and empowerment regarding the production process and the machines they operate.

Similarly, SUP are considered another CSF for QUA, as they provide raw materials in the required quantity and time and convey essential information, facilitating production process operations [19]. SUP constitute the foundation on which the QUA of a product is constructed. Therefore, meticulous selection and effective management of SUP must be conducted to ensure that they meet the required technical and sustainable standards. Consequently, close collaboration between the manufacturer and its SUP is necessary for the identification and resolution of QUA-related issues, and to reduce costs due to waste and rejections that affect customer satisfaction and increase expenses. Thus, SUP should be regarded as strategic allies that enable manufacturers to guarantee a reliable and durable product that meets market expectations.

However, SUP and OPE can only generate a QUA through an efficient production process that requires calibrated machines that do not generate waste or rework. In this production process, other LMTs that support QUA are implemented, such as Kaizen, which focuses on continuous improvement and waste reduction; 5S, because a clean and organized workplace identifies QUA problems, reduces errors, and improves delivery times; poka-yoke, which prevents errors by incorporating devices into machines and tools; Kanban as a visual aid to improve the flow of materials and to perform only the required activities; TPM to calibrate machines; and a value stream map (VSM) to compare the system states before and after an intervention [20], among others. Therefore, the following hypotheses are proposed:

H_4. Operators have a direct and positive effect on the QUA of the production process.

H_5. Suppliers have a direct and positive effect on the QUA of the production process.

H_6. Lean manufacturing tools implemented in the production process have a direct and positive effect on the QUA obtained.

The relationships between the variables established as hypotheses are shown in Figure 1.

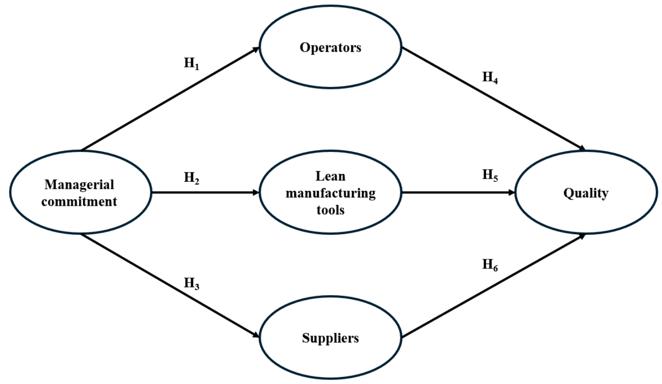

Figure 1. Proposed hypotheses

III. MATERIALS AND METHODS

A. Stage 1. Design of a questionnaire

To validate the hypotheses, data are required from managers, engineers, and individuals associated with the supply chain who oversee OPE in the Mexican Maquiladora industry. The variables in Figure 1 are latent and can be elucidated using other observed variables (items). A comprehensive literature review was conducted to identify previous studies in which these variables were analyzed, facilitating the development of an initial questionnaire. This questionnaire was subsequently validated in a geographical context by a panel of judges who evaluated aspects pertaining to the clarity and precision of the items, their relevance, coherence, and neutrality [21].

The final questionnaire was reviewed and the Institutional Commission on Research Ethics and Bioethics oversaw the project to ensure compliance with the Helsinki Agreement. The questionnaire comprised three sections: the first inquired about demographic aspects; the second investigated the critical success factors of QUA; and the third examined the benefits of QUA. While the first section of the questionnaire was optional, the second and third sections utilized a 5-point Likert scale (1-5) for responses.

B. Stage 2. Application of the questionnaire

The Google Forms platform was utilized to administer an online questionnaire to managers and engineers who had a minimum of one year of experience in their respective positions and had implemented QUA projects, which were required to be concluded to enable the evaluation of the benefits and results. An electronic mail containing a hyperlink to the online questionnaire was sent to potential respondents; however, two additional questions were incorporated. The initial question inquired about respondents' willingness to participate in the research and their agreement with the academic and scientific use of the information. In the event of disagreement, the questionnaire was terminated without further response. The questionnaire was accessible between March 1 and June 1, 2024.

C. Stage 3. Debugging and validation of the information

Upon completion of the questionnaire application period, a data file was extracted from the response database and subjected to a cleaning process comprising the following procedures [22]:

1. Identification of non-committed respondents through standardization of each questionnaire.

2. Detection of missing values. Cases exhibiting more than 10 % of missing data were excluded from the analysis, whereas those with lower percentages were imputed using the median.

3. Identification of extreme values through standardization of each item, with subsequent replacement by the median.

Following the data-cleaning process, the latent variables were validated using the indices proposed by Kock [23]. These indices included R^2 and adjusted R^2 for parametric predictive validity, composite reliability index, Cronbach's alpha index for internal validation, average variance extracted for convergent validity, variance inflation indices for multicollinearity, and Q^2 for nonparametric predictive validity.

D. Stage 4. Descriptive analysis of the items

Descriptive analyses were conducted using SPSS v.22 software. To elucidate the contribution of each item to its corresponding latent variable, the median was calculated as a measure of central tendency and the interquartile range (IQ) was determined as a measure of dispersion, given that the data were collected on an ordinal scale. Elevated median values indicated a high frequency of these activities, whereas lower values suggested a less frequent occurrence. Similarly, higher interquartile range values denote a lack of consensus regarding the item's median value, whereas lower values indicate a high degree of consensus or agreement among respondents.

E. Stage 5. Structural equation modeling

The structural equation modeling (SEM) technique was selected to validate the hypotheses because of its capacity to evaluate the relationship between latent variables integrated by items (as observed in this study) that can simultaneously function as dependent and independent variables. In this investigation, SEM was assessed using a partial least squares (PLS) approach, which is recommended for ordinal scales and small samples and does not necessitate the fulfillment of normality in variables. PLS-SEM is useful in predictive research where formative and reglective constructs exist, was used to evaluate social sustainability and manufacturing leadership [24] and to evaluate the impact of LMT on social sustainability [25].

The PLS-SEM analysis was conducted using WarpPLS v.8 software. Prior to interpreting the results, a series of indices that the model must satisfy were examined, including the average of the coefficients, average R2, and average adjusted R2 to measure the predictive validity of the model. Additionally, the averages of the variance inflation indices were calculated to assess collinearity, and the Tenenhaus index was used to measure the fit of the data to the model [23].

In the SEM analysis, three effects or relationships between variables were obtained, measured using a standardized parameter β as a measure of dependence, and their statistical significance was determined with a 95 % confidence level [26]. For each effect, the effect size (ES) is reported as a measure of the variance explained by the independent variable in the dependent variable. Furthermore, the R^2 value was associated with each dependent variable. Initially, the direct effects that enable the validation of the proposed hypotheses are reported; subsequently, the indirect effects that occur through the mediating variables are presented; and finally, the total effects, which comprise the sum of the direct and indirect effects, are reported.

F. Step 6: Sensitivity analysis

To determine the risks of having low levels of implementation in some of the variables and their items, three probabilities were reported in this study, which were obtained using WarpPLS v.8 software:

- Probability that a latent variable occurs at a high or low isolation level.
- Probability that two latent variables co-occur jointly in their combinations of high and low levels.
- The conditional probability that the dependent latent variable will occur at a high or low level given that the independent variable has occurred at one of its high or low levels.

IV. RESULTS

A. Descriptive analysis of the sample

A total of 1345 emails containing the questionnaire link were distributed to potential respondents, resulting in 312 responses, representing a response rate of 23.19 %. During the data filtering process, 26 responses were excluded due to a high percentage of missing data, leaving 286 responses for the analysis. Table 1 indicates that most respondents were male, experienced managers, and engineers, with the automotive sector being the most representative industry.

Table 2 presents the medians and interquartile ranges for the analyzed items, with four items exhibiting higher medians and three in the QUA variable, emphasizing MAC's culture of change and teamwork. For OPE, QUA assurance requires that they are responsible for inspecting their work and are adequately trained to make decisions that enhance product QUA. Regarding LMTs, it is primarily required that processes are standardized and errors are prevented; SUP are required to be certified and to maintain long-term relationships. Finally, the success of the QUA programs is demonstrated through the implementation of TQM and established metrics.

TABLE I
SAMPLE DATA

Category	Quantity	Percentage
	Sex	
Man	193	67.48
Woman	93	32.52
	Job position	
Manager	127	44.41

Engineer	112	39.16
Supervisor	47	16.43
Years in position		
1-2	20	6.99
2-5	49	17.13
5-10	86	30.07
>10	131	45.80
Industrial sectors		
Automotive	123	43.01
Electric	62	21.68
Electronic	48	16.78
Textile	27	9.44
Machining	14	4.90
Physician	12	4.20

TABLE II
DESCRIPTIVE ANALYSIS OF THE ITEMS

Management Commitment (MAC)	M	RI
The organization has a culture that fosters change.	3.58	1.72
Supervisors strive to foster teamwork by encouraging operators to cooperate and express their opinions.	3.54	1.71
Managers, engineers and operators constantly interact with each other.	3.54	1.61
The different departments of the plant are coordinated and in constant communication.	3.51	1.58
There is support and commitment from management in the execution of JIT.	3.48	1.51
Operators (OPE)		
Operators are responsible for inspecting their work.	3.70	1.65
Employees are trained to perform multiple tasks.	3.60	1.83
There are work teams to solve production problems and encourage employee participation.	3.57	1.76
Emphasis is placed on improving workers' skills and knowledge.	3.53	1.58
Many problems are solved by getting suggestions from workers.	3.52	1.76
Employees are hired for their ability to solve problems and work as part of a team.	3.47	1.72
Lean manufacturing tools (LMT)		
Processes are standardized.	3.68	1.60
A device to avoid errors (Poka-Yoke) has been implemented.	3.67	1.61
The design of the installation is product oriented.	3.66	1.55
The layout design is process oriented.	3.59	1.70
Suppliers (SUP)		
The company's suppliers are certified.	4.05	1.61
The company has long-term contracts with its suppliers.	3.76	1.56
Deliveries are received daily from most suppliers.	3.50	1.70
Suppliers are integrated into the company through a pull system.	3.47	1.78
QUA (QUA)		
Total QUA Management (TQM) principles and tools have been implemented.	4.21	1.57
QUA metrics are in place	4.17	1.60
A total productive maintenance (TPM) program has been implemented.	4.04	1.66
QUA initiatives are customer oriented.	3.96	1.59
Statistical control is used to control and reduce process variation.	3.90	1.72

B. Validation of the variables and the model

Table 3 presents the validation indices for the latent variables. As demonstrated in the final column, all the indices meet the minimum requirement. This indicates that sufficient parametric, nonparametric internal, and convergent predictive validity were present, and the variables exhibited no collinearity issues.

TABLE III
VALIDATION OF LATENT VARIABLES

Index	QUA	SUP	LMT	MAC	OPE	Best if
R^2	0.44	0.12	0.10		0.25	>0.02
R^2 Adjusted	0.43	0.12	0.09		0.25	>0.02
CRI	0.93	0.88	0.84	0.88	0.86	>0.7
CA	0.91	0.82	0.76	0.83	0.81	>0.7
AVE	0.73	0.66	0.58	0.60	0.51	>0.5
VIF	1.69	1.85	1.68	1.33	1.45	<3.3
Q^2	0.44	0.12	0.10		0.25	>0

CRI=Composite reliability index, CA=Cronbach's alpha, AVE= Average variance extracted, VIF=Variance inflation index

The validated variables were incorporated into the Structural Equation Model (SEM), and the efficiency indices demonstrated that the model exhibited adequate internal validity, possessed predictive capability, and lacked collinearity among the latent variables. Consequently, we proceeded with the interpretation of the SEM. The model indices are:

- Average path coefficient (APC)=0.329, P<0.001
- Average R-squared (ARS)=0.231, P<0.001
- Average adjusted R-squared (AARS)=0.227, P<0.001
- Average block VIF (AVIF)=1.441, ideally <= 3.3
- Average full collinearity VIF (AFVIF)=1.605, ideally <= 3.3
- Tenenhaus GoF (GoF)=0.378, large >= 0.36

C. Structural equation model

Figure 2 illustrates the PLS-SEM evaluated in WarpPLS 8.0, wherein the β value, associated p-value, and effect size (ES) of each direct effect proposed in Figure 1 as hypotheses are presented. Based on the p-values associated with the β parameters, it was determined that all hypotheses were accepted as they were less than 0.05.

In this investigation, there was only an indirect effect of MAC on QUA, with β=0.292, through the mediating variables OPE, LMT, and SUP, which were statistically significant at P<0.001.

As these two variables exhibited no direct effect, this indirect effect constituted the total effect between them in this study.

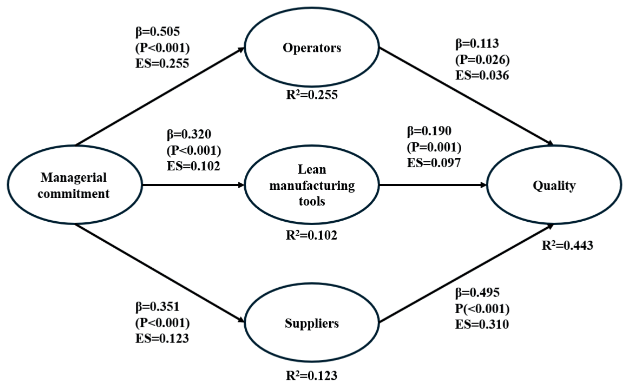

Figure 2. Evaluated model - validation of hypothesis

D. Sensitivity analysis

In WarpPLS v.8 software, the probabilities of occurrence were estimated for the variables. In this study, the probability that a variable is implemented adequately and efficiently is denoted when it has a standardized value greater than one, that is, P(Z>1), and is represented by the "+" sign. Conversely, the probability that a variable is implemented inadequately or inefficiently is denoted when the standardized value is less than minus one, that is, P(Z<-1), and is represented by the "-" sign. Table 4 illustrates the probabilities of the variables occurring independently and jointly, represented by "&", while the conditional probability is represented by "IF".

V. DISCUSSION OF RESULTS

Several conclusions and inferences can be drawn from the SEM and sensitivity analyses. The results indicate that MAC directly and positively affects OPE (H_1), with β=0.505, explaining up to 25.5 % of its variability. Furthermore, when MAC+ occurs, the probability of OPE+ occurring is 0.326, while the probability of OPE- is 0.000, as Li and Griffin [27]. Conversely, if MAC- occurs, there is a probability of OPE- of 0.281, which represents a significant risk in production lines, where OPE- does not contribute to the resolution of QUA issues and MAC- is only weakly associated with OPE+, with a probability of 0.094. A low MAC level directly affects the low commitment of OPE+, limiting managers' opportunities to integrate OPE+ perspectives for continuous improvement.

Similarly, the analysis demonstrated that MAC directly and positively affected LMT (H_2), with β=0.320, explaining up to 10.2 % of its variability. The occurrence of MAC+ favors the occurrence of LMT+ with a probability of 0.348, whereas the probability of LMT-is only 0.109. Effective manufacturing practices in the production process depend on managers who possess the decision-making authority to authorize process modifications. However, if MAC- occurs, indicating that managers are not integrated into the production process, LMT- can occur with a probability of 0.219, and LMT+ with a probability of 0.094. This suggests that production processes may be deficient, unproductive, and disorganized in the presence of limited MAC, which negatively impacts the product's final QUA and, according to García-Alcaraz, *et al.* [28], constitutes a high risk.

TABLE IV
SENSITIVITY ANALYSIS

Variable	Probability	MAC+	MAC-	OPE+	OPE-	LMT+	LMT+	SUP+	SUP-
		0.161	0.112	0.178	0.143	0.164	0.161	0.182	0.143
OPE+	0.178	&=0.052 IF=0.326	&=0.010 IF=0.094						
OPE-	0.143	&=0.000 IF=0.000	&=0.031 IF=0.281						
LMT+	0.164	&=0.056 IF=0.348	&=0.010 IF=0.094						
LMT-	0.161	&=0.017 IF=0.109	&=0.024 IF=0.219						
SUP+	0.182	&=0.063 IF=0.391	&=0.007 IF=0.063						
SUP-	0.143	&=0.017 IF=0.109	&=0.028 IF=0.250						
QUA+	0.133	&=0.035 IF=0.217	&=0.010 IF=0.094	&=0.028 IF=0.157	&=0.007 IF=0.049	&=0.031 IF=0.191	&=0.024 IF=0.152	&=0.031 IF=0.173	&=0.000 IF=0.000
QUA-	0.154	&=0.021 IF=0.130	&=0.028 IF=0.250	&=0.024 IF=0.137	&=0.045 IF=0.317	&=0.000 IF=0.000	&=0.059 IF=0.370	&=0.010 IF=0.058	&=0.073 IF=0.512

MAC also exhibited a direct and positive effect on SUP (H_3), with β=0.351, explaining up to 12.3 % of its variability. The significance of MAC on SUP is evident, as the occurrence of MAC+ is associated with a probability of 0.391 for SUP+ and only 0.109 for SUP −. This indicates that a positive relationship between managers and SUP fosters long-lasting trusting relationships contributing to QUA. However, MAC- is associated with SUP- with a probability of 0.250 and is only weakly associated with SUP+ with a probability of 0.063, suggesting that managers who are not committed to integrating SUP into their production processes generate limited communication, lack of coordination, and insufficient joint commitment to QUA.

The results further indicate that OPE directly and positively affect QUA (H_4) with β=0.113, explaining 3.6 % of its variability. The relatively small percentage may be attributed to OPE' limited decision-making authority, as they execute QUA plans and programs from the administration without aligning with SUP. If OPE+ occurs, QUA+ can occur with a probability of 0.157 and QUA- with a probability of 0.137, which are notably similar. This similarity may be due to the significant dependence of QUA on SUP in the Mexican Maquiladora industry. Similarly, if OPE- occurs, there is a risk of QUA- with a probability of 0.317, and QUA+ with a probability of 0.049.

Structural equation modeling (SEM) analysis revealed that LMT exhibits a direct and positive effect on QUA (H_5) with β=0.190, accounting for 9.7 % of its variability. Furthermore, the occurrence of LMT+ is associated with a 0.192 probability of QUA+ occurrence, whereas the conditional probability of QUA+ given LMT- is 0.000. This finding suggests that implementing LMT supporting QUA consistently yields benefits in production lines and is economically advantageous [29]. Conversely, the occurrence of LMT- was associated with probabilities of 0.370 and 0.152 for QUA- and QUA+, respectively.

The analysis indicates that SUP directly affects QUA, with β=0.495 (H_6), explaining 31.0 % of QUA variability, representing the second-largest effect in the analyzed model. Moreover, the occurrence of SUP+ was associated with probabilities of 0.173 and 0.058 for QUA+ and QUA-, respectively. The integration and co-responsibility of SUP in the manufacturer's production process enhances the manufacturer's QUA [30]. Conversely, their non-integration poses a risk that managers should avoid, as SUP- occurrence is associated with a 0.512 probability of QUA- occurrence and a 0.000 probability of QUA+ occurrence. This finding underscores that SUP integration consistently promotes QUA.

Although MAC does not directly relate to QUA, it demonstrates an indirect effect through OPE, LMT, and SUP, with β=0.292, accounting for 7 % of QUA variability. This relationship is corroborated by the observation that MAC+ occurrence is associated with probabilities of 0.217 and 0.130 for QUA+ and QUA −, respectively. This indicates that even with MAC+, QUA- remains possible owing to the involvement of the OPE, LMT, and SUP. Additionally, MAC- occurrence was associated with probabilities of 0.250 and 0.094 for QUA- and QUA+, respectively. These results suggest that MAC not only supports OPE, LMT, and SUP but also contributes to QUA by promoting the implementation of QUA assurance plans and programs and facilitating the allocation of necessary resources and supervision of their appropriate utilization.

VI. CONCLUSIONS AND INDUSTRIAL IMPLICATIONS

This study provides substantive evidence for the critical role of MAC in enhancing QUA and economic sustainability within the manufacturing industry. Through the application of a SEM, significant relationships between MAC and key operational factors—OPE, SUP, and LMT—have been identified. These findings offer valuable insights for managers and decision-makers seeking to improve their quality management practices and overall sustainability. The key conclusions are as follows:

MAC as a cornerstone: The results demonstrate that MAC serves as the foundation for an integrated quality management system. While MAC does not directly affect QUA, it exerts a substantial indirect effect (β = 0.292) through its influence on OPE, SUP, and LMT. This underscores the pivotal role of leadership in creating an environment conducive to quality improvement and sustainability.

SUP integration: The study reveals that SUP has the strongest direct effect on QUA (β = 0.495), explaining 31 % of its variability. This highlights the critical importance of effective SUP relationships in achieving and maintaining high-quality standards.

OPE empowerment: Although OPE has a smaller direct effect on QUA (β = 0.113), their role is essential in implementing quality protocols and identifying potential issues at the source. Empowering operators through training and involvement in decision-making processes can significantly enhance their contribution to quality outcomes.

LMT positively affects QUA (β = 0.190), accounting for 9.7 % of its variability. This emphasizes the importance of implementing lean practices to optimize processes, reduce waste, and improve efficiency.

These conclusions have several industrial implications and practical applications, including:

Cultivating leadership for QUA: Managers must prioritize their commitment to QUA initiatives, as this establishes the foundation for the entire organization. This can be achieved by implementing regular leadership development programs focused on quality management principles, establishing clear quality objectives, communicating them consistently across all levels of the organization, and allocating resources specifically for QUA improvement projects and initiatives.

Enhancing SUP relationships: Given SUP's significant impact on QUA, managers should focus on developing long-term, collaborative partnerships with key SUP, implementing joint QUA assurance programs and certifications with SUP, establishing clear communication channels and shared quality standards with SUP, and organizing regular SUP forums or exhibitions to foster innovation and alignment with QUA goals.

Empowering operators to leverage the potential of OPE in quality management, wherein managers should implement comprehensive training programs that focus on quality control techniques and problem-solving methodologies, establish operator-led quality circles or improvement teams to facilitate active participation in quality initiatives, and develop a suggestion system that incentivizes operators for identifying and resolving quality issues.

To optimize LMT, managers should conduct a thorough assessment of current processes to identify areas for lean implementation, prioritize the adoption of key lean tools such as 5S, Kaizen, and poka-yoke to standardize processes and mitigate errors, and implement visual management systems to enhance accessibility of quality standards and performance metrics for all employees.

Integrating quality management systems and managers should develop an integrated quality management framework that aligns MAC, OPE, SUP, and LMT initiatives. Additionally, they should implement cross-functional teams to oversee quality improvement projects, ensure collaboration between various departments, and utilize operational analytics and AI technologies to monitor quality metrics and identify areas for improvement in real time.

Finally, managers need to foster a culture of continuous improvement by establishing regular review processes to assess the efficacy of quality management practices, facilitate knowledge sharing and dissemination of best practices across the organization, and recognize and reward employees and teams that contribute significantly to quality improvement and sustainability efforts.

VII. LIMITATIONS AND FUTURE RESEARCH

While this study provides valuable insights, further research is necessary to expand our understanding of quality management and sustainability in industrial contexts. Future investigations should explore additional critical success factors, such as specific leadership styles and their impact on quality management effectiveness, examine the role of targeted training programs for operators and their influence on quality outcomes and sustainability, investigate how the integration of emerging technologies (e.g., Industry 4.0, AI, IoT) can enhance quality management practices and sustainability efforts, and conduct longitudinal studies to assess the long-term impact of managerial commitment on quality and sustainability performance. Furthermore, the applicability of these findings across diverse industrial sectors and cultural contexts should be explored to develop more generalizable insights.

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Numerical Study Using CFD on Heat Sinks for Electronic Components

Fernando Toapanta-Ramos[1], Javier Espin[2], and William Diaz[3]

Abstract — **In the present study, a numerical investigation is carried out using ANSYS CFD to observe the heat transfer and heat dissipation, the method is by forced convection heat transfer, with a modern and innovative heat sink. In the study, a configuration of six vertical central fins of equal size and three small fins horizontally is observed. With the lower surface heated, this simulates the heat rejection of electronic devices such as video cards in CPUs. The Navier-Stokes equations for fluid dynamics and the Kappa-Epsilon turbulence model based on RNG (Renormalization) are established for this study. The temperature in the air surrounding the heat sink increases by 0.62 to 0.79 °C, for the base temperature of 80 °C and 100 °C, respectively. This means that at a higher air flow speed, 20 m/s, the air has the capacity to heat up more since its heat exchange is stronger, therefore, the heat sink reduces its temperature.**

Keywords: **Heat sink; CFD; temperature; heat transfer.**

Resumen — **En el presente estudio, se lleva a cabo una investigación numérica mediante CFD de ANSYS para observar la transferencia de calor y la disipación de calor, el método es por transferencia de calor por convección forzada, con un disipador moderno e innovador. En este estudio se observa una configuración de seis aletas centrales verticales de igual medida y tres aletas pequeñas de forma horizontal. Con la superficie inferior calentada, con esto se simula el rechazo de calor de dispositivos electrónicos como tarjetas de video en CPU's. Las ecuaciones de Navier-Stokes para la dinámica de fluidos y el modelo de turbulencia Kappa-Épsilon basado en RNG (Renormalización) se establecen para este estudio. La temperatura en el aire que mueve hasta el disipador de calor aumenta entre 0.62 y 0.79 °C, para la temperatura en la base de 80 °C y 100 °C, respectivamente, esto se traduce que a mayor velocidad de flujo de aire, 20 m/s, el aire tiene la capacidad de calentarse más ya que su intercambio de calor es más fuerte, por lo tanto, el disipador de calor reduce su temperatura.**

Palabras Clave: **Disipador de calor; CFD; temperatura; transferencia de calor.**

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I. INTRODUCTION

NOWADAYS, the components of high and medium efficiency computer equipment generate a significant amount of heat, due to the fact that the speed of data processing is increasing, which makes it imperative to use elements that allow heat dissipation, to prevent overheating, which causes defects and damage to the integrity of computers and the information they store.

Due to rapid progress in electronic device technology, there is a growing need for solutions to evacuate the generated heat. A new design explored how the thermal dynamics inside the heat sink changes by modifying the angles of the secondary branches to 45 and 90 °C and adjusting the opening widths [1].

The study by Kepekci and Asma [2] has found that the fin geometry is one of the most important factors causing the pressure loss of the heat sinks during operation. Based on the results, the airfoil configuration is determined as the arrangement of fins to the geometry of the heat sink.

The use of air-cooled microchannel heat sinks is becoming more and more widespread for cooling supercomputers. Air passing through microchannels, which acts as an absorber, is the main heat transfer mechanism for cooling the main board of supercomputers. The results showed that among the five channel configurations, the triangular shape provides the highest thermal performance for cooling a specific microchannel heat sink. However, with respect to manufacturing cost, the straight-fee configuration is recommended [3].

Through multiple investigations that attempted to calculate the heat transfer rate from the surface of the heat sink, many of them focused on the configuration of the fins and microchannels in reference to the inlet shape [4], [5].

In the numerical study conducted by Sultan et al. [6] they found that, the velocity contours indicate that the openings have the significant effect of allowing heat to transfer from the hot layer to the outer air layers, which is the main mechanism used to evacuate the heat generated by natural convection cooling.

Bakhti and Si-Ameur [7] analyzed the performance of elliptical fin heat sinks in a mixed convection scenario. They observed that, there is an optimal aspect ratio where heat dissipation is maximum.

The results of the CFD simulation show that the rectangular fins have a better overall cooling effect on the heat source. And the double-row aligned rectangular fin arrangement under the condition of inlet 1 has the best heat dissipation ability on the hot side of the thermoelectric cooler, with 2.92% better heat dissipation than other rectangular fin cases on average [8].

Numerical simulations were performed to evaluate the heat transfer efficiency of a vertical heat sink with curved fins with different thickness aspect ratios, the continuity, momentum, and energy equations were solved using FLUENT, the study concluded that the volume occupied by classical fins can be reduced by up to 57.8% if curved fins are adopted [9].

Abbas & Wang [10] they opted to use a new fin offset design to increase heat dissipation by unforced convection without increasing volume. The simulation results showed that the heat sink has a rate of thermal transfer improvement 30%, a 28.7% reduction in total mass, and a 27.4% reduction in surface area compared to a conventional heat sink.

Huang and Chen [11] investigated the performance of a plate-fin heat sink under the influence of natural convection experimentally and with simulations. They analyzed three different configurations of the plate-fin heat sink considering variations in fin height and fin offsets in the lateral direction. These researchers recommended that the configurations are suitable for practical applications as a result of their superior cooling performance and ease of fabrication.

Siddhartha et al. [12] performed numerical investigations to analyze the heat transfer performance of circumferential fins. It was observed that the average Nusselt number increased with an increase in the number of cycles. Furthermore, they also observed that increase in fin diameter leads to an increase in the average Nusselt number.

Al-Damook et al. [13] studied the thermal performance of pin-fin heat sinks under the influence of forced convection considering a turbulent flow model. They compared solid pin-fins with perforated pin-fins and found that pin-fins with 5 perforations resulted in 11% higher Nu values compared to solid pin-fins.

The performance of the curved fin model and the straight fin model are comparable. The minimum temperature reached by the straight fin model is 1.26 °C lower than that reached by the curved fin model, at maximum engine speed, showing that this is due to the surface area provided by the straight fin model being larger than the surface area of the curved fin model [14].

For forced convection, as the Reynolds number increases the Nusselt number, heat transfer rates and pressure drop also increases. Fins with perforation, slot, corrugated, dimples, notch, and interruption for either free or forced conditions showed a better heat transfer rate than the solid fins. Staggered arrangement for a pin fin, flat fin, perforations, and slots showed good enhancement in heat transfer coefficient compared to the inline arrangement. The spacing between fins had a significant influence on the heat sink performance [15].

At lowest Re = 13049, the Nusselt numbers of the arrowhead with perforation, hexagonal with perforation and concave with perforation are increased by 16.0%, 12.2% and 0.288% respectively over the solid novel fin. At highest Re = 52195, the Nusselt numbers of the arrowhead with perforation, hexagonal with perforation and concave with perforation are increased by 34.28%, 44.07% and 27.48% respectively over the solid novel fin [16].

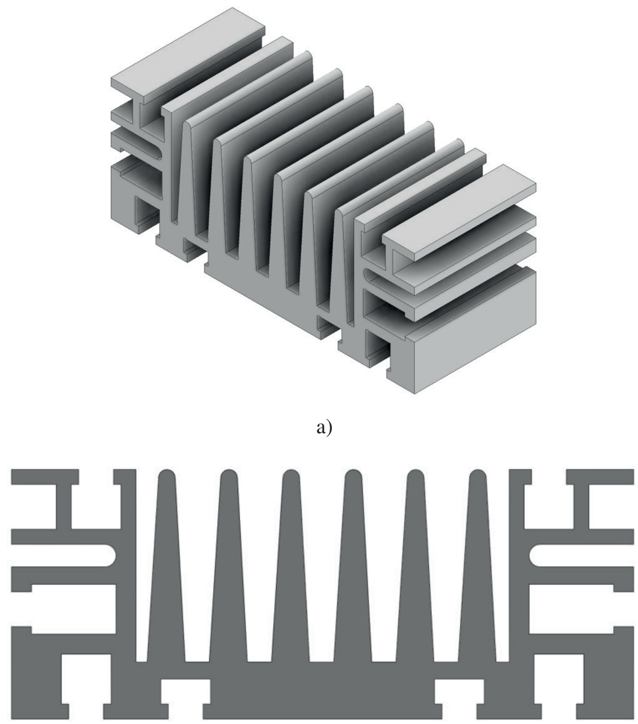
The objective of this research is to determine the temperature dissipation when using a heat rejection system, by means of a special heat sink. The study focuses on numerical simulation with CFD (computational fluid dynamics) for the cooling of computer systems.

II. METHODS AND MATERIALS

Heat sinks used in computer systems are usually made of aluminum or aluminum alloys. Many researchers [17], [18] have used this type of material for their studies.

The designed heatsink has several features such as: its dimensions are small, 50 mm wide, 50 mm high and 125 mm long, in figure 1a the heatsink can be seen in three dimensions, while figure 1b is the front representation of the heatsink. With attachments at the bottom for attachment to the computer structure, this heatsink is capable of cooling devices such as video cards or processing cards.

The type of heat sink fins are triangular fins in the center of the device, which run along its entire width. There are also other rectangular fins on each side of the heat sink, which are perpendicular to the triangular fins.



a)

b)

Fig. 1. Heat sink, a) 3D view and b) front view.

The heat sink has six main fins for heat rejection, in addition to other extended surfaces that help dissipation, however, it is presumed that it will not influence as much as the main fins.

Cooling is carried out by a forced convection heat transfer process, with a cross-air flow of 10 m/s and another of 20 m/s.

The lower heating temperature, which is the surface close to the video card, has temperatures ranging from 80 °C to 100 °C, so simulations are performed with these temperatures to verify the temperature reduction in extreme cases of heating.

Since this is a numerical study with CFD, it is absolutely necessary to carry out a study of the mesh, in order to determine the best mesh, both in the heat sink and in the air. Under this approach, it is necessary to find the ideal number of nodes and elements that demonstrate that the mesh has a low obliquity.

Figure 2 represents the analysis of heat transfer. Two parts are observed, the first is the heat sink and the other is the air surrounding the heat sink, the latter represents the air that passes through the cross-flow heat sink.

The hot surface at the bottom of the heatsink is always the first area that the heat flow from the video card reaches, and through it the electronic system cools down.

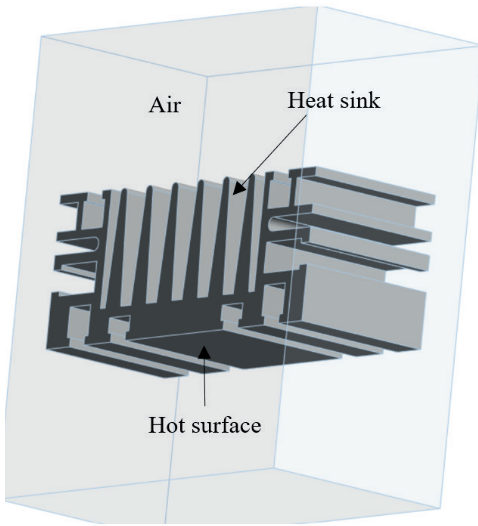


Fig. 2. Cross flow heat dissipation system.

In Figure 3, the mesh convergence in the heat sink can be observed, taking into account that there are three types of meshes such as tetrahedrons, and hexahedrons, and octahedrons, the latter two having a smaller number of elements. Both elements and nodes are distributed in the mesh, there are 482729 and 97216, respectively. However, the most important thing is the quality of the mesh, having an average obliquity of 0.285, this corresponds to a good mesh for the simulations that are performed.

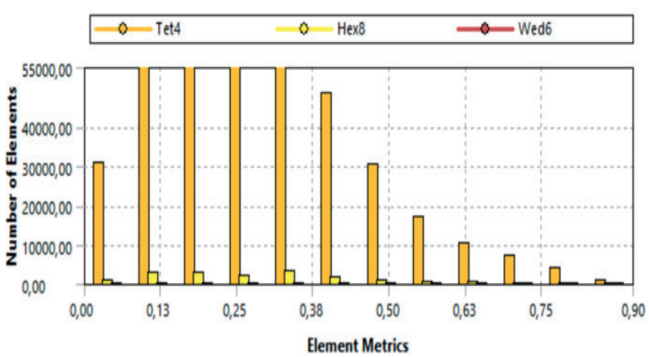


Fig. 3. Mesh convergence.

In CFD simulation, the continuity, momentum and energy equations govern the turbulent, Newtonian [19], [20], [21] incompressible airflow with heat transfer through a plate-fin heat sink. To do this, it is essential to know which equations are used in the heat transfer system by heat dissipation.

Continuity equation, as shown in Eq. 1.

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}=0 \tag{1}$$

Momentum equations,
X-Momentum, as shown in Eq. 2:

$$\rho\left[u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}+w\frac{\partial u}{\partial z}\right]=-\frac{\partial p}{\partial x}+\mu\left[\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right] \tag{2}$$

Y-Momentum, as shown in Eq. 3:

$$\rho\left[u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}+w\frac{\partial v}{\partial z}\right]=-\frac{\partial p}{\partial y}+\mu\left[\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}+\frac{\partial^2 v}{\partial z^2}\right] \tag{3}$$

Z-Momentum, as shown in Eq. 4:

$$\rho\left[u\frac{\partial w}{\partial x}+v\frac{\partial w}{\partial y}+w\frac{\partial w}{\partial z}\right]=-\frac{\partial p}{\partial z}+\mu\left[\frac{\partial^2 w}{\partial x^2}+\frac{\partial^2 w}{\partial y^2}+\frac{\partial^2 w}{\partial z^2}\right] \tag{4}$$

Energy equation, as shown in Eq. 5,

$$u\frac{\partial T}{\partial x}+v\frac{\partial T}{\partial y}+w\frac{\partial T}{\partial z}=\frac{K_f}{pC}\left[\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}\right] \tag{5}$$

The Kappa-Epsilon model is used for the current simulations. Heat transfer in heat sinks under the effects of cross air flow are simulated and can be predicted under this viscosity model. This model has ideal characteristics for heat transfer performance [22].

Kappa equation, as shown in Eq. 6,

$$\begin{aligned}&\frac{\partial}{\partial t}(\rho\kappa)+\frac{\partial}{\partial x_i}(\rho\kappa u_i)=\\&\quad\frac{\partial}{\partial x_j}\left[\alpha_k\mu_{eff}\frac{\partial k}{\partial x_j}\right]+G_k+G_b-\rho\epsilon-Y_M+S_\kappa\end{aligned} \tag{6}$$

Epsilon equation, as shown in Eq. 7,

$$\begin{aligned}&\frac{\partial}{\partial t}(\rho\epsilon)+\frac{\partial}{\partial x_i}(\rho\epsilon u_1)=\frac{\partial}{\partial x_j}\left(\alpha_\epsilon u_{eff}\frac{\partial\epsilon}{\partial x_j}\right)\\&\quad+C_{1\epsilon}\frac{\epsilon}{\kappa}(G_\kappa+C_{3\epsilon}G_b)-C_{2\epsilon}\rho\frac{\epsilon^2}{\kappa}-R_\epsilon+S_\epsilon\end{aligned} \tag{7}$$

Using the numerical heat transfer model, it is necessary to determine how the heat flux rises from the base to the fins of the heat sink through the surrounding air. The numerical analysis is carried out for different velocities in a range from 10 m/s to 20 m/s. At these velocities a fully developed turbulent Reynolds number is reached. The variation of air properties due to temperature is not considered in this analysis. The density and viscosity of the air are considered as constants.

To determine the heat flow released by the heat sink, it is necessary to find out whether the flow is in laminar or turbulent regime; for this, it is essential to determine the Reynolds number, as shown in Eq. 8, using equation 8.

$$Re = \frac{\rho_{air} U_{air} D_h}{\mu_{air}} \tag{8}$$

Convection heat flux is taken as the main means of heat transfer therefore, as shown in Eq. 9 is used to determine the outgoing heat flux.

$$\dot{Q}_c = h_p A_p (T_s - T_a) \tag{9}$$

The heat convective coefficient, as shown in Eq. 10, can be obtained by rearranging equation 9.

$$h_p = \frac{\dot{Q}_c}{A_p \left[T_s - \frac{T_{out}+T_{in}}{2}\right]} \tag{10}$$

Figure 4 represents the mesh to be used in the heat dissipation system, where the air flow mesh and the fins that make up the heat sink are located.

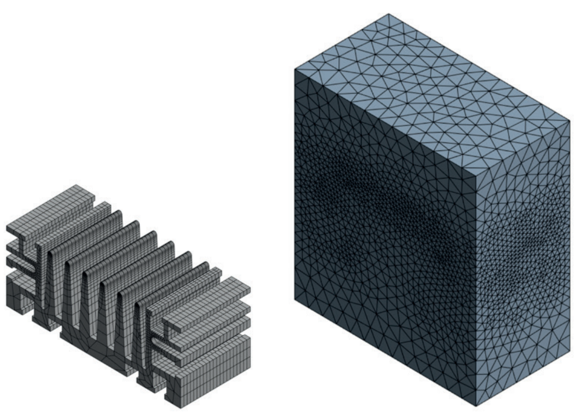
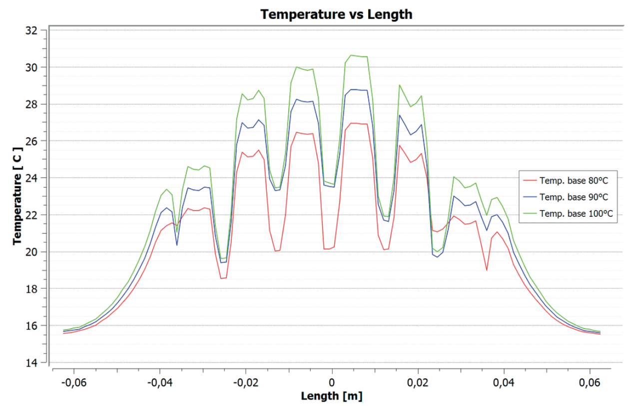


Fig. 4. Meshing of the heat sink and surrounding air.

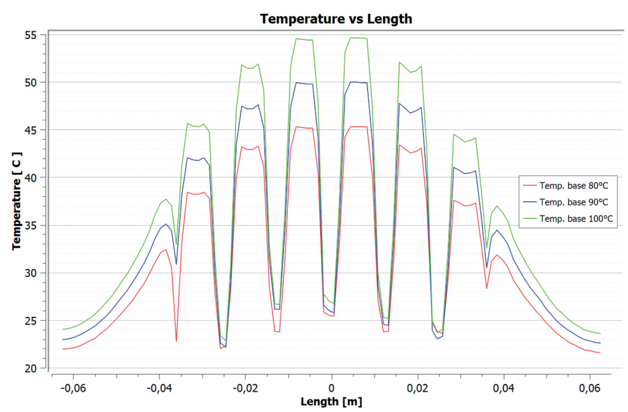
III. RESULTS

First, it is determined how the temperature increases as time passes. Figure 5 shows how the temperature increases when it is measured at half the height of the heat sink. These simulation times are 2 s, 5 s and 10 s. Figure 5a shows that the high temperature peak is at 30.5 °C in the central fin, when the base temperature is 100 °C, the temperature decreases when the base temperature is modified, this simulation corresponds to 2 s. On the other hand, Figure 5b shows a similar behavior, since the highest temperature reaches 55 °C and the lowest reaches 27 °C, in the same fin. In the same way, Figure 5c represents the temperature of the heat sink at 10 s, reaching a maximum and minimum value of 75 °C and 61 °C, respectively.

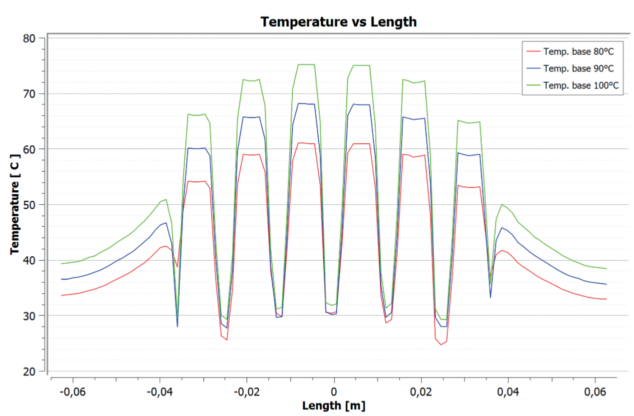
Figure 6 shows two temperature contours on the heat sink, the one on the top corresponds to the base temperature of 80 °C, while the one on the bottom is the heat sink with a base temperature of 100 °C, this at an air speed of 10 m/s and with a simulation time of 10 s. It can be seen that, the heat rises through the body of the heat sink, taking the heat with it and reducing the temperature of the electronic computational device.



a)



b)



c)

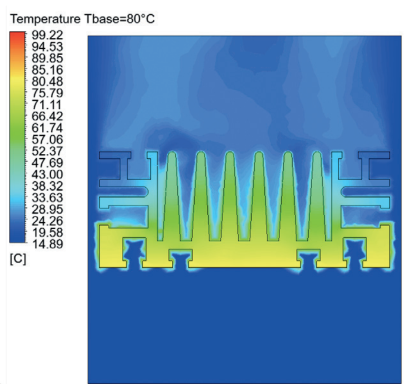
Fig. 5. Comparative results at air speed of 10 m/s: a) time 2 s, b) time 5 s and c) time 10 s.}

Similarly, it is seen that the air surrounding the heat sink also increases its temperature, when the base temperature is 80 °C the temperature in the upper space reaches 24.62 °C and for the base temperature of 100 °C, in the environment it reaches 26.45 °C, there is an increase of 7.34%, which means that when having an increase of 20 °C in the base temperature the surrounding air barely rises 2 °C, therefore, the heat sink is operating under its thermal design standards.

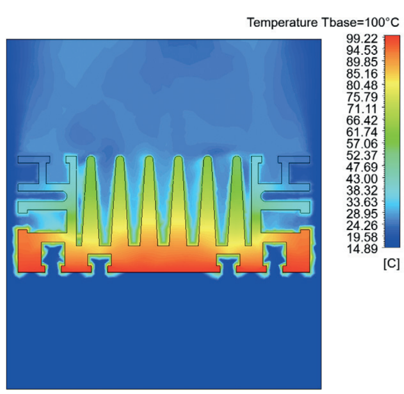
On the other hand, it is seen that heat dissipation occurs mostly through the main fins, the fins on the sides collaborate in the elimination, however, they do not help greatly in the rejection of heat, this is an argument to understand that the side fins are only for the support and fixation of the heat sink.

Figure 7 represents the speed of the air that is circulating around the heat sink, for the two analysis speeds 10 m/s and 20 m/s, where it can be seen how the air flow lines affect the increase or decrease in temperature throughout the heat sink. The results presented in this figure correspond to a base temperature of 90 °C.

In Figure 7a, an isometric view of the air flow is displayed, taking into account that for the sector of 20 m/s in inlet speed, it tends to accelerate, due to its geometric configuration, up to a maximum of 90.28 m/s, this improves the heat transfer, since a forced convective medium helps the space tend to decrease the temperature, when compared to a non-forced medium. Similarly, it is observed that the air speed increases on the front and back faces, as well as at the vertices of the heat sink.



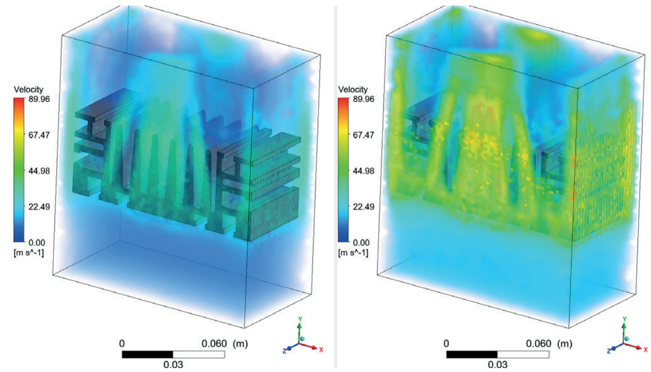
a)



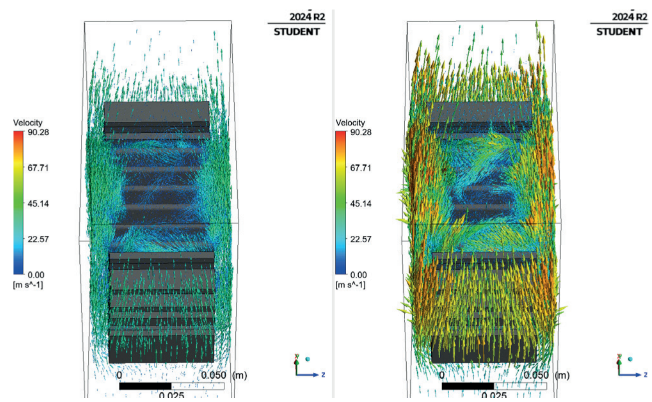
b)

Fig. 6. Heat flow in the heat sink a) Base temperature 80 °C and b) Base temperature 100 °C.

On the other hand, figure 7b compares the two cases of the inlet velocity, 10 m/s and 20 m/s, however, in a top view of the heat sink, it is observed that the air flow tends to enter through the central part of the device, through the main fins, which causes heat transfer by forced convective flow to occur there, in the 10 m/s section there is little air flow entering, however, in the 20 m/s section the air flow increases and it enters in greater quantity to the central fins of the heat sink.



a)



b)

Fig. 7. Velocity vectors around the heat sink at 10 m/s and 20 m/s a) Isometric view and b) top view.

The study of the heat sink is about numerically verifying the rejection of heat by means of fins, however, this analysis is carried out in a transitory manner, in other words, taking into account the simulation time, for this reason, several simulations are carried out as a function of time.

Figure 8 is a representation of two analysis cases, at a constant base temperature of 100 °C with the two speeds studied. The reference for data collection is located in the upper central part of the heat sink. However, the times of 2 s, 5 s and 8 s are taken as reference to determine whether the temperature increases or decreases when passing through the heat sink.

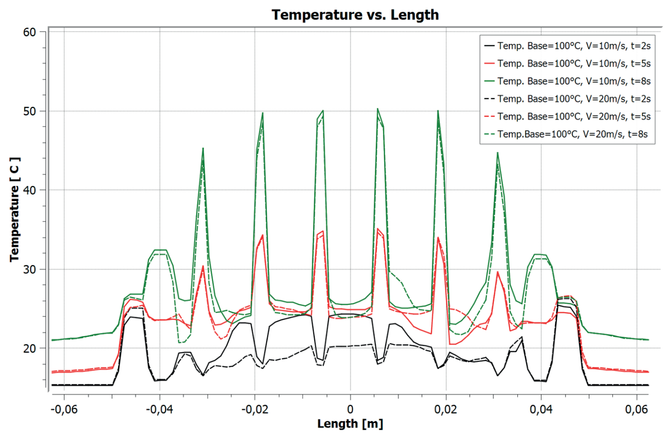


Fig. 8. Temperature variation in the heat sink at times of 2s, 5s and 8s, for speeds of 10 m/s and 20 m/s.

The results found in figure 8 are the following: when comparing the air temperature just at the heat sink outlet, at time 2 s there is a higher temperature for the case of 20 m/s in speed, there is an increase of 5 °C in the space between fins, however, when it is in the fin the temperature decreases to 18 °C for the speed of 10 m/s and increases 0.5 °C, for twice the speed.

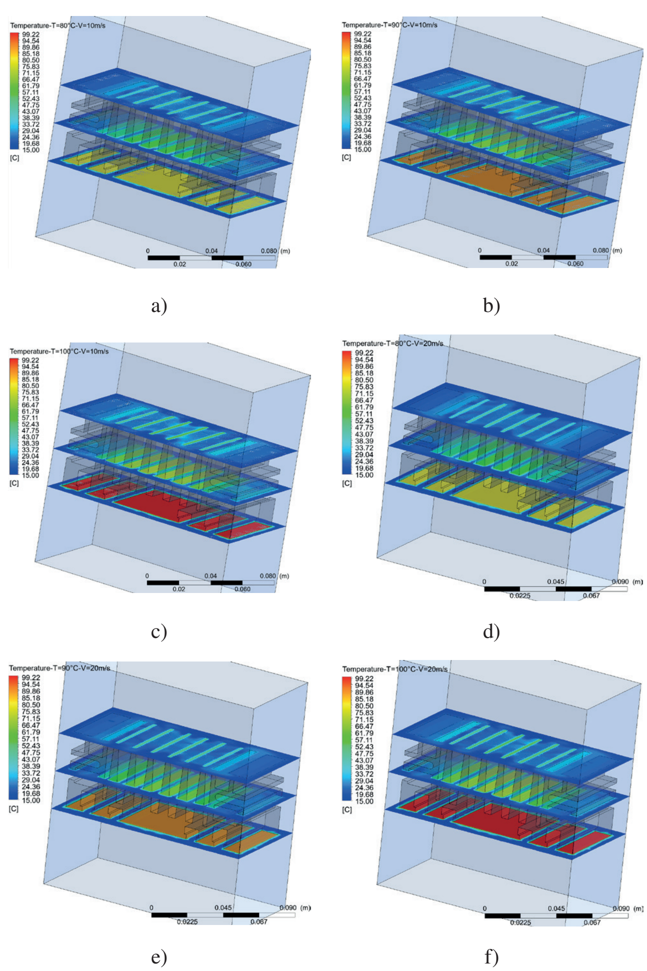


Fig. 9. Temperature contour, upper, central and lower part of the fin, a) T=80 °C, V=10 m/s; b) T=90 °C, V=10 m/s; c) T=100 °C, V=10 m/s; d) T=80 °C, V=20 m/s; e) T=90 °C, V=20 m/s; f) T=100 °C, V=20 m/s

The other way around, for a time of 5 s and the same variables as in the previous case, the air temperature in the spaces between the fins remains stable around 25 °C, the change occurs in the fins, which tend to heat up, which is what is expected with heat sinks, since the temperature rises through the structure of the fin. In this case, the maximum temperature reached is 35 °C for a speed of 10 m/s and 34 °C for a speed of 20 m/s. There is a small variation which shows that the central part of the heat sink does not receive the air flow to improve heat transfer. In the upcoming results, different positions inside the heat sink will be evaluated.

The last case of analysis, in figure 8, shows the purchase at time 8 s, here it is observed that the temperature rises to 50 °C at a speed of 20 m/s and decreases 0.5 °C when reducing the speed by half. This is in the section where there are fins, for the empty spaces between fins the temperature is between 22 °C and 25 °C.

Figure 9 shows six different results for the heat sink a, b, and c are temperature results around the heat sink with an initial speed of 10 m/s, with temperatures of 80 °C, 90 °C, and 100 °C, respectively. On the other hand, results d, e, and f are for an initial speed of 20 m/s, under the premise of the same three temperatures evaluated.

The six sub-figures, corresponding to figure 9, are temperature results in three different positions of the heat sink, at the top, middle and bottom of it. In all of them it can be seen that the temperature around the heat sink is at 15 °C, which is the air inlet temperature, both for 10 m/s and 20 m/s. The results of the upper part always have low temperatures and in the lower part temperatures close to the base temperature.

Figure 9a represents the heat distribution along the heat sink, this is reflected by the temperature in the three positions, marking 49.33 °C at the top in the central fins and decreasing in the vicinity until reaching 15 °C, while in the central position the temperature reaches 61.5 °C in the central fin. While in the outer fin the temperature reaches 52.78 °C, this is due to the fact that there is a greater amount of air.

Figure 9d is the result of heat dissipation under the same circumstances as the case of figure 9a, however, there is a change in speed to 20 m/s. Here it can be seen that the temperature at the top of the heat sink reaches 48.14 °C, there is a reduction of 2.47%, it is not as large as expected. Something similar happens in the middle part of the heat sink, since there is a maximum temperature in that position of 60.64 °C, with a percentage decrease of 1.41 %. Similarly, in the outer fin the temperature is 51.82 °C, reducing by 1.85 %.

Figures 9b and 9e are the temperature results for the heat sink, for a base temperature of 90 °C, with velocities of 10 m/s and 20 m/s, respectively. In part b, the temperatures are 54.62 °C, 68.72 °C and 58.56 °C, for the sectors of the upper central part, in the middle part of the central fin and in the middle part of an extreme fin, respectively. On the other hand, the result of part e, in the same previous positions are 53.13 °C, 67.61 °C, and 54.45 °C. These temperatures correspond to the air speed of 20 m/s. Despite the fact that the base temperature increased by 10 °C, the temperature at the top barely increased by 5.29 °C, and 4.99 °C for the two analysis speeds, which confirms that the increase in speed does improve heat transfer.

Finally, Figures 9c and 9d are the results for the heat sink with the base temperature of 100 °C. Again, the two airflow velocities are 10 m/s and 20 m/s. The results presented in these simulations for the first velocity are 59.85 °C, 75.87 °C, and 65.74 °C, for the upper, central, and outer fin sectors, respectively. On the other hand, at the 20 m/s velocity, the temperatures in the same sectors are 58.15 °C, 74.60 °C, and 64.29 °C, respectively. Even though the temperature in any of the cases decreases only 1 °C, it is a reduction and the behavior of the electronic device will improve its availability.

In Figure 10a, the two analysis lines on the heat sink can be seen, the data collection line which is located in the middle of the fin and crosses along the z axis, and the air line which is the data collection in the space between the fins, in the same way along the same axis.

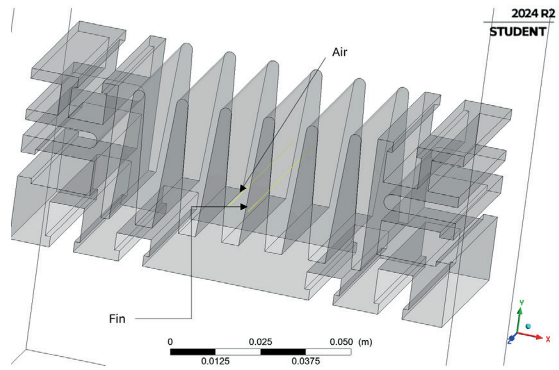
Figure 10b, denotes the temperatures in the two analysis positions, both in the air between the fins and the central fin, the analysis speed is 10 m/s. It can be seen that in the region of the central fin the temperatures reach 78 °C and the minimum of 62 °C, for the two simulated temperature extremes at the base 100 °C and 80 °C, respectively. On the other hand, the results of the air temperature in the section between the fins are visualized in the lower part of the figure, here the maximum temperature is 36 °C and 30 °C as a minimum. However, a reduction in temperature in the central part of the z axis, this represents that in that section the air is not transferring heat as it does in the corners of the heat sink.

Figure 10c, finally, is the representation of the temperature in the two sections of analysis, air between the fins and the central fin. In this figure, a decrease of 2 °C is visualized in the central fin, this due to the increase in the speed of the air to 20 m/s. While in the space between the fins, the maximum and minimum temperatures are 40 °C and 28 °C, respectively. In the same way, there is the same amount of decrease in temperature.

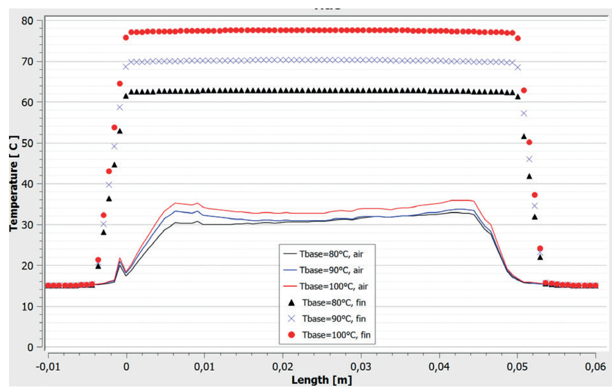
IV. CONCLUSIONS

In the present study, three-dimensional CFD simulations were analyzed for transient flow conditions where the airflow is turbulent. The air velocity has been modified as well as the base temperature of the heat sink, six simulations were compared, three with a velocity of 10 m/s and three with 20 m/s. The main results are summarized as follows:

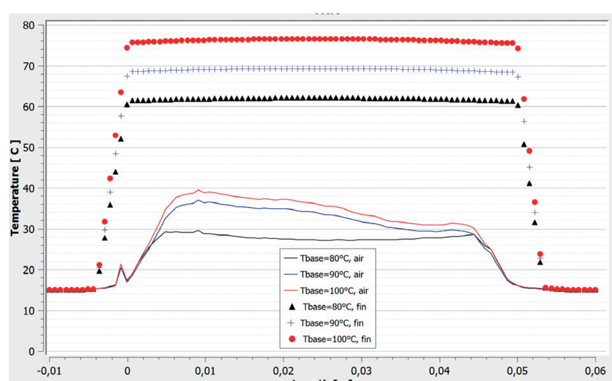
- The heat sink temperature is reduced when the device encounters a change in airflow around it. For the three base temperatures analyzed, the temperature at the end of the center fin is 50.869 °C, and 56.136 °C, and 61.549 °C, respectively. When increasing the base temperature from 80 °C to 90 °C, it was found that there is an increase of 10.35 % in the analysis section, meanwhile, when increasing from 90 °C to 100 °C, it increases by 9.64 % with respect to the previous temperature. These values are results for the speed of 10 m/s.
- Similarly, when comparing the temperatures, at the same position, for the two analysis speeds, with the base temperature unchanged, it was found that there is a decrease in temperature of 1,411 °C, and 1,354 °C, and 1,543 °C, for base temperatures of 80 °C, and 90 °C, and 100 °C, respectively.
- Finally, the temperature in the space between the fins, where there is only air, does not vary much, even though the temperature at the base increases from 80 °C to 100 °C, from 24,901 °C to 26,953 °C. Meanwhile, the difference in temperature in the air between the two speeds does not exceed 0.8 °C.



a)



b)



c)

Fig. 10. Temperature on the z axis, analysis on the fin and the space between fins, a) Lines for taking results, b) V=10 m/s and c) V=20 m/s.

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