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Kinetic Study Of Acetylene Hydrogenation Reaction To Improve The Efficiency Of Ethylene Production Process

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Summary

A documentary review was carried out on the production and publication of research papers related to the study of the variables Acetylene Hydrogenation and Ethylene Production. The purpose of the bibliometric analysis proposed in this document was to know the main characteristics of the volume of publications registered in the Scopus database during the period 2017-2022, achieving the identification of 44 publications in total. The information provided by this platform was organized through graphs and figures, categorizing the information by Year of Publication, Country of Origin, Area of Knowledge and Type of Publication. Once these characteristics have been described, the position of different authors on the proposed topic is referenced through a qualitative analysis. Among the main findings made through this research, it is found that China, with 21 publications, was the country with the highest scientific production registered in the name of authors affiliated with institutions of that nation. The Area of Knowledge that made the greatest contribution to the construction of bibliographic material related to the study, productivity, innovation and their levels within the local markets was Chemical Engineering, with 27 published documents, and the Type of Publication that was most used during the period indicated above was the Journal Article, which represents 86% of the total scientific production.

Key words: *Acetylene Hydrogenation, Ethylene Production, Literature Review.*

1. Introduction

The acetylene hydrogenation reaction plays an important role in the petrochemical industry as it serves the purpose of optimizing and efficient ethylene production processes. Ethene, a chemical compound made up of two carbon atoms linked by two bonds, is considered to be one of the most important chemicals in this industry. Likewise, the hydrogenation of acetylene poses several inconsistencies,[1] since the presence of acetylene is a highly reactive impurity, hindering efficiency in ethylene production processes. Incorporating hydrogenation plays a key role in minimizing challenges at the time of production, as it improves processes, improves efficiency, and ensures high-quality ethene production.

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Acetylene or ethylene is the simplest alkyne. It is a gas, highly flammable, slightly lighter than air and colorless, is thermodynamically unstable and can cause detrimental effects on the ethylene production process. Their interaction can lead to a shock on the surfaces of the catalyst, which would cause the deactivation of the catalyst, compromising the performance of ethylene. Knowing the characteristics and difficulties that acetylene presents, poor production can produce undesired negative effects, resulting in operational problems and higher production cost, effective removal of acetylene is imperative to maintain the economic viability and sustainability of ethylene production.

The usual targets of this reaction are unsaturated organic compounds, such as alkenes, alkynes, ketones converting them into more stable and saturated forms. The production of ethylene, the hydrogenation process is carried out by means of catalyzed systems, these systems are essential in the production processes since they must exhibit a high selectivity towards the conversion of acetylene and thus reduce the secondary effects of this ethylene and guarantee a long life of the catalyst.

Several catalyst systems have been implemented for acetylene hydrogenation processes, among these palladium-based systems have been used, which has high properties of activity and selectivity. These catalysts operate under mild conditions, providing an efficient means of selectively removing acetylene without affecting other hydrocarbons present in the feedstock. It is worth mentioning that advances in the efficiency of these catalysts are still in constant evolution, as it is expected that better efficiency processes in hydrogenation will be gradually available. Ensuring the optimization mechanisms in the tempering and pressure parameters through acetylene correlation is an aspect to be taken into account since this guarantees the success of this hydrogenation reaction. Adjusting these parameters is essential to achieve optimal acetylene conversion rates while minimizing energy consumption and operating costs. Advances in process engineering and reactor design contribute significantly to the overall efficiency of the hydrogenation process. For this reason, this article seeks to describe the main characteristics of the compendium of publications indexed in the Scopus database related to the variables Acetylene Hydrogenation and Ethylene Production, as well. Such as the description of the position of certain authors affiliated with institutions, during the period between 2017 and 2022.

2. General Objective

To analyze, from a bibliometric and bibliographic perspective, the production of research papers on the variables Acetylene Hydrogenation and Ethylene Production recorded in Scopus during the period 2017-2022.

3. Methodology

A quantitative analysis of the information provided by Scopus is carried out under a bibliometric approach on the scientific production related to the study of Acetylene Hydrogenation and Ethylene Production. Likewise, from a qualitative perspective, examples of some research works published in the area of study mentioned above are analyzed, from a bibliographic approach to describe the position of different authors regarding the proposed topic.

The search is carried out through the tool provided by Scopus and parameters referenced in Figure 1 are established.

3.1 Methodological design

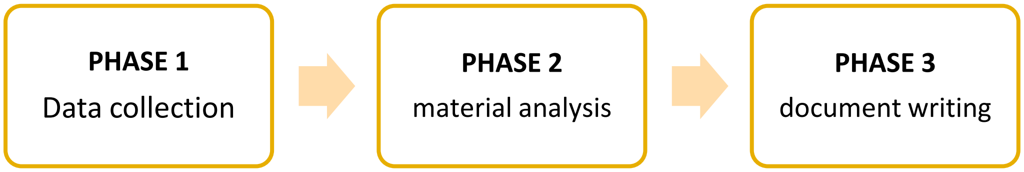

Figure 1. Methodological design
Source: Authors.

3.1.1 Phase 1: Data collection

Data collection was carried out through the Search tool on the Scopus website, through which a total of 44 publications were identified. To this end, search filters were established consisting of:

TITLE-ABS-KEY (acetylene AND hydrogenation, AND ethylene AND production) AND PUBYEAR > 2016 AND PUBYEAR < 2023

- ✓ Published documents whose study variables are related to the study of Acetylene Hydrogenation and Ethylene Production
- ✓ Without distinction of country of origin.
- ✓ Without distinction of area of knowledge.
- ✓ No distinction of type of publication.

3.1.2 Phase 2: Construction of analytical material

The information identified in the previous phase is organized. The classification will be made by means of graphs, figures and tables based on data provided by Scopus.

- ✓ Co-occurrence of Words.
- ✓ Year of publication
- ✓ Country of origin of the publication.
- ✓ Area of knowledge.
- ✓ Publication Type

3.1.3 Phase 3: Drafting of conclusions and outcome document

After the analysis carried out in the previous phase, we proceed to the drafting of the conclusions and preparation of the final document.

4. Results

4.1 Co-occurrence of words

Figure 2 shows the co-occurrence of keywords within the publications identified in the Scopus database.

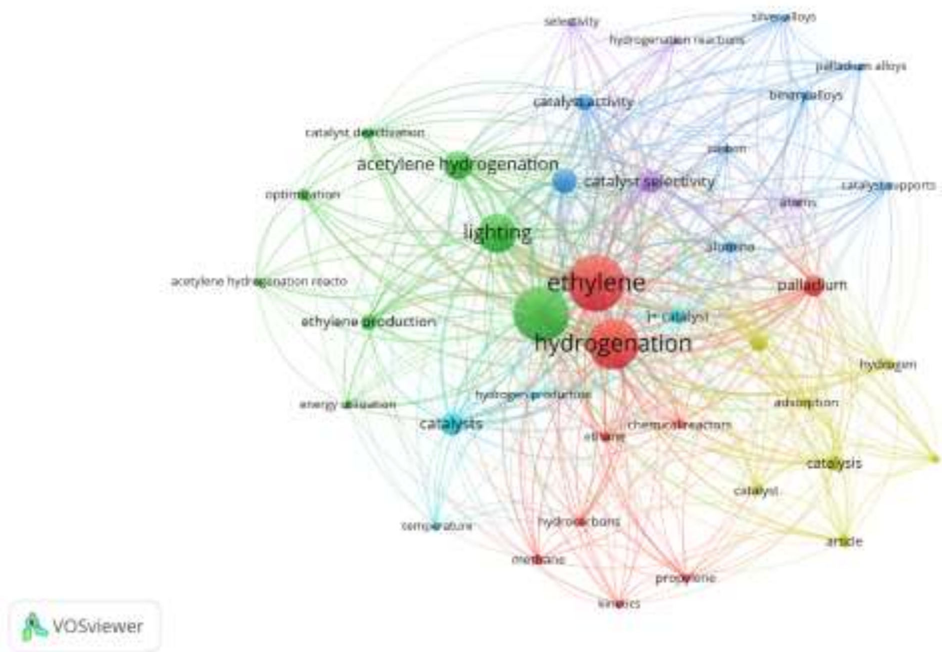

Figure 2. Co-occurrence of words
Source: Authors' own elaboration (2022); based on data provided by Scopus.

Hydrogenation was the most frequently used keyword within the studies identified through the execution of Phase 1 of the Methodological Design proposed for the development of this article. Ethylene is among the most frequently used variables, associated with variables such as Acetylene Hydrogenation, Ethylene Production, Hydrocarbons, Temperature, Hydrogen Production, Catalyst Selectivity, Palladium. This comprehensive exploration of acetylene hydrogenation within the ethylene production process underscores the intricate balance required to achieve high efficiency, profitability, and environmental sustainability. As the global demand for ethylene continues to increase, the development of innovative technologies and the continuous refinement of hydrogenation processes become imperative to ensure a reliable and sustainable supply of this essential component for the petrochemical industry. In the following sections, we will delve into the mechanisms, catalytic systems, and technological advances that drive acetylene hydrogenation, shedding light on ongoing efforts to optimize this critical step in ethylene production.

4.2 Distribution of scientific production by year of publication.

Figure 3 shows how scientific production is distributed according to the year of publication, taking into account that the period between 2017 and 2021 is taken

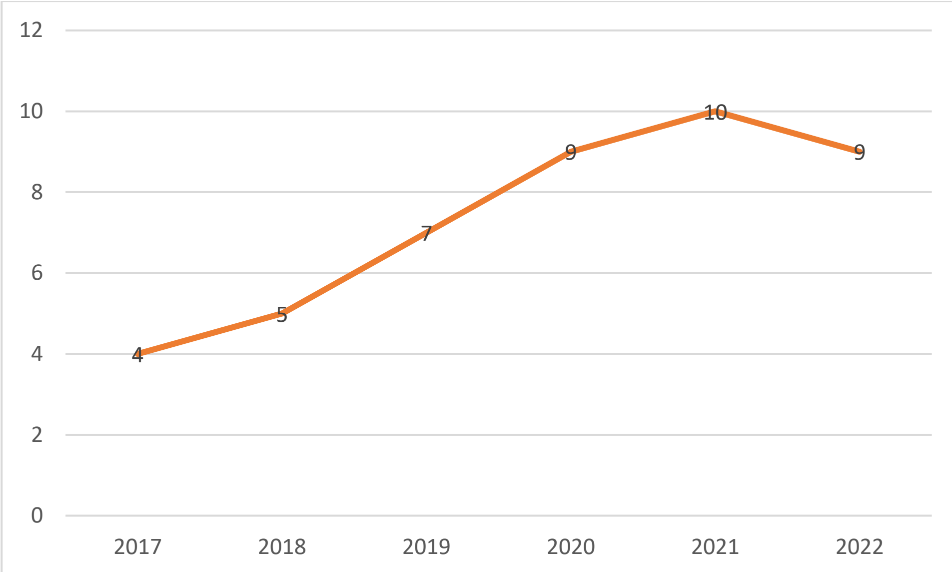

Figure 3. Distribution of scientific production by year of publication.
Source: Authors' own elaboration (2022); based on data provided by Scopus.

Among the main characteristics evidenced through the distribution of scientific production by year of publication, the level of number of publications registered in Scopus was in 2021, reaching a total of 10 documents published in journals indexed on this platform. This can be explained by articles such as the one titled "Optimization of the complete cycle of acetylene conversion distribution for a serial reactor of acetylene hydrogenation beds", this article first considers the effect of temperature on the accumulation of green oil and corrects the kinetic equation of catalyst deactivation. Second, to ensure that the temperature in each reactor bed is within the most suitable temperature range for the reaction, two distribution schemes of the acetylene conversion rate in each reactor bed are provided from the perspectives of chemical reaction engineering theory and safety. in the actual production process. Finally, the acetylene conversion rate constraint is added to the conventional full-cycle operation optimization model, the acetylene conversion rate distribution full-cycle operation optimization model is established, and two acetylene conversion rate distribution schemes are optimized. The optimization results show that the ethylene yield optimized by the two acetylene conversion distribution schemes is much higher than that optimized by conventional operation, and the ethylene yield is higher when the acetylene conversion scheme is 33(Wang, 2022): 33: 33. Considering the safety in the actual production process, the distribution scheme of acetylene conversion is 43:47:10, which has a better result.

4.3 Distribution of scientific production by country of origin.

Figure 4 shows how the scientific production is distributed according to the nationality of the authors.

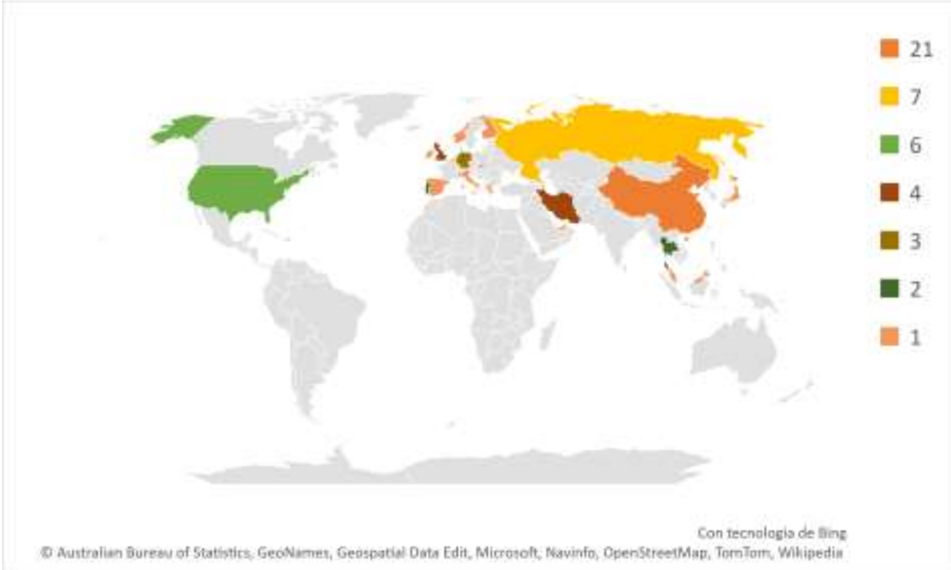

Figure 4. Distribution of scientific production by country of origin.
Source: Authors' own elaboration (2022); based on data provided by Scopus.

Within the distribution of scientific production by country of origin, the registrations from institutions were taken into account, establishing China as the country of this community, with the highest number of publications indexed in Scopus during the period 2017-2022, with a total of 21 publications in total. In second place, Russia with 7 scientific papers, and the United States taking third place presenting to the scientific community, with a total of 6 papers among which is the article entitled "Machine learning-assisted catalytic yield predictions of single-atom alloys for acetylene semihydrogenation" In this paper, we established a pioneering machine learning (ML)-assisted approach to investigate the reaction activity and selectivity of 70 SAA catalysts for acetylene semihydrogenation. As the most desirable ML model, the gradient increase regression (GBR) algorithm has been extended to predict the energy barrier of *C2Hn(n = 2-4) hydrogenation with a mean square error (RMSE) of only 0.02 eV. In particular, five candidate SAAs with excellent activity and selectivity for acetylene semi-hydrogenation are selected using accessible descriptors. These ML prediction data have been verified by DFT calculation with high accuracy (error less than 0.07 eV). This work demonstrates the potential of the ML-assisted approach to predict the energy barrier of the transition state and at the same time provides a convenient approach for the rational design of efficient catalysts.(Feng, 2022)

4.4 Distribution of scientific production by area of knowledge

Figure 5 shows how the production of scientific publications is distributed according to the area of knowledge through which the different research methodologies are executed.

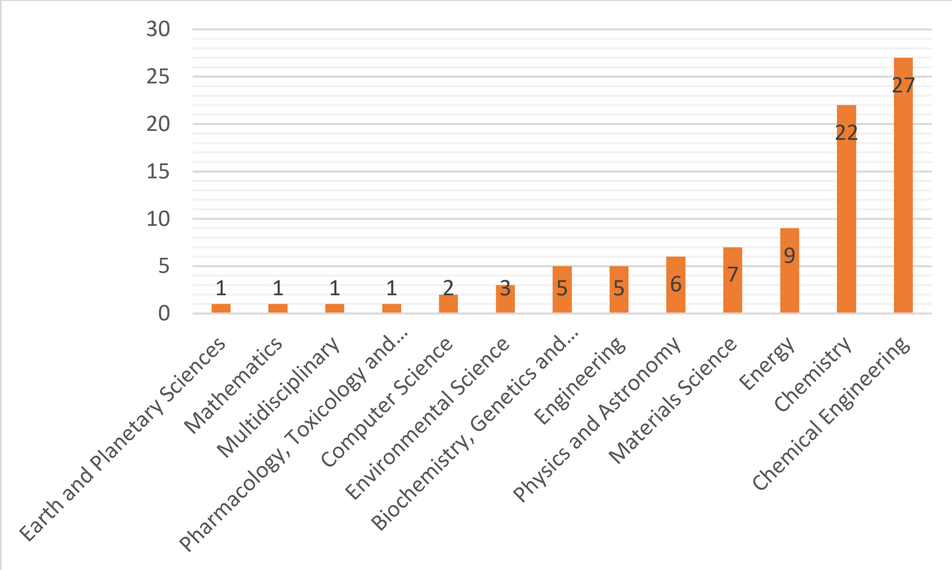

Figure 5. Distribution of scientific production by area of knowledge.
Source: Authors' own elaboration (2022); based on data provided by Scopus.

Chemical Engineering was the area of knowledge with the highest number of publications registered in Scopus with a total of 27 documents that have based its methodologies Acetylene Hydrogenation and Ethylene Production. In second place, Chemistry with 22 articles and Energy in third place with 9. The above can be explained thanks to the contribution and study of different branches, the article with the greatest impact was registered by Chemical Engineering entitled "Identification of copper as an ideal catalyst for the electrochemical semihydrogenation of alkynes" In this paper, we present an atomic understanding of the trend in electrocatalytic semihydrogenation of acetylene in 12 transition metals with systematic calculations of the density functional theory and the model of the hydrogen electrode. Copper stands out and is theoretically identified as the ideal metal for electrocatalytic conversion of acetylene to ethylene with a suppressed hydrogen release reaction. Our theoretically predicted Cu catalyst has been successfully synthesized and experimentally proven to be superior for selective semi-hydrogenation of alkynes, which largely validates our computational framework for rational catalyst design. This work not only illustrates the key factors that determine activity and selectivity, but also provides new suggestions for further optimization of this environmentally benign and economically viable pathway for the semi-hydrogenation of environmental alkynes.(Chen, 2022)

4.5 Type of publication

Figure 6 shows how the bibliography is distributed according to the type of publication chosen by the authors

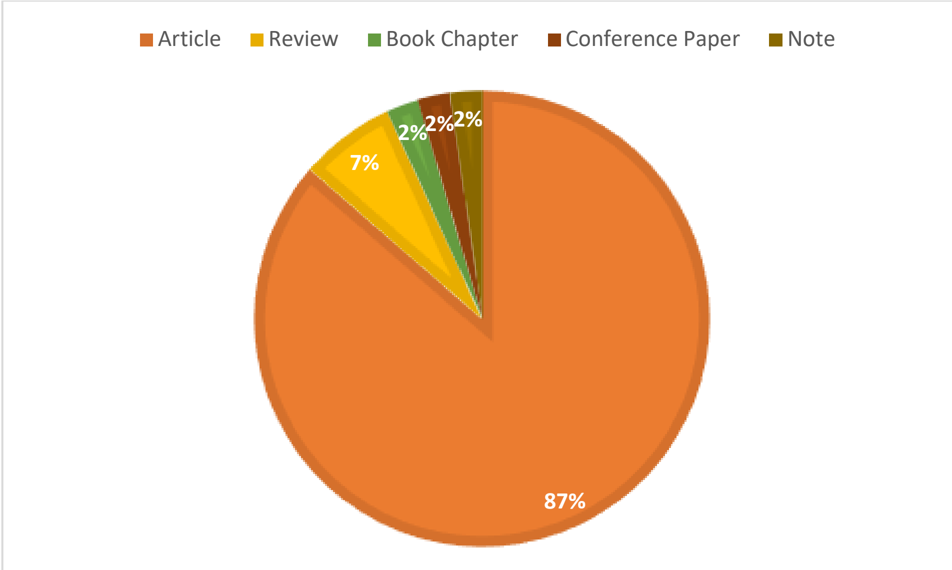

Figure 6. Publication Type
Source: Authors' own elaboration (2022); based on data provided by Scopus.

The type of publication most frequently used by the researchers referenced in the body of this document was the one entitled Journal Articles with 87% of the total production identified for analysis, followed by Journal with 7%. Chapter of the Book are part of this classification, representing 2% of the research papers published during the period 2017-2022, in journals indexed in Scopus. In this last category, the one entitled "Effect of hydrogen pretreatment on the structure and properties of carbon-supported Pd-Ag nanoalloys for the production of ethylene by acetylene hydrogenation stands out" The process of formation of the active component of 0.5%Pd-0.5%Ag catalysts supported on the pyrolytic carbon black/synthetic carbon compound "Sibunit" was studied. which were synthesized by co-impregnation. XRD and EXAFS studies revealed that heating the Pd-Ag/Sibunit catalyst in hydrogen to 400–500 °C results in the formation of a solid bimetallic solution Pd0.6Ag0.4. Bimetallic particles are characterized by a greater distance between neighboring palladium atoms (2.78-2.80 Å) compared to metallic palladium and by an increase in the electron density of palladium atoms under the action of silver (according to XPS data). Samples synthesized with supported Pd-Ag nanoparticles allow C2H4 to be obtained by ethine hydrogenation with a selectivity of 77 to 78%.(Glyzdova, 2021)

5. Conclusions

Through the bibliometric analysis carried out in this research work, it was established that China was the country with the highest number of published records regarding the variables Acetylene Hydrogenation and Ethylene Production. With a total of 21 publications in the Scopus database. In the same way, it was established that the application of theories framed in the area of Chemical Engineering, were used more frequently in the hydrogenation reaction of acetylene, since this chemical transformation, in which acetylene is converted into ethylene through the addition of hydrogen, is not simply an industrial process; This transformative approach goes further and derives a holistic horizon for the optimization and reduction of production costs in general. The importance of ethylene in the global chemical industry cannot be underestimated, as it serves as a critical component for a wide range of products, including plastics, solvents, and various organic chemicals. Traditional methods for ethylene production processes require hydrocarbon steam processes, but hydrogenation-scale research provides this industry with a different and more efficient alternative focus. The incorporation of this reaction has proven to be particularly beneficial in addressing the challenges associated with acetylene impurities, which can compromise ethylene quality and yield. The main advantages of employing acetylene hydrogenation lie in its ability to selectively convert acetylene into ethylene, thereby eliminating undesirable byproducts that may arise from other methods. This specific role not only improves the purity of the final ethylene product, but also minimizes waste, contributing to a more sustainable and environmentally friendly production process. Acetylene hydrogenation offers better control over reaction parameters, allowing for better regulation of temperature, pressure, and catalyst activity. Proper control of it is critical to optimize the efficiency and selectivity of the reaction, which ultimately leads to higher ethylene yields. The use of advanced catalysts and reaction engineering has further contributed to the development of highly efficient and cost-effective hydrogenation processes. ignore the environmental impact of ethylene production, and acetylene hydrogenation aligns with the industry's growing focus on sustainability. By reducing the release of unwanted by-products and optimising resource utilisation, this process contributes to a more environmentally responsible approach to ethylene manufacturing. Advances in catalyst technology continue to drive the development of more sustainable and energy-efficient hydrogenation processes.

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