World Journal of Advanced Research and Reviews
eISSN: 2581-9615 CODEN (USA): WJARAI
Cross Ref DOI: 10.30574/wjarr
Journal homepage: https://wjarr.com/

(RESEARCH ARTICLE)

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Effect of catalyst composition on the hydrogenation efficiency and product yield in the catalytic degradation of polyethylene terephthalate

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World Journal of Advanced Research and Reviews, 2024, 21(01), 2951-2958

Publication history: Received on 19 November 2023; revised on 07 January 2024; accepted on 09 January 2024

Article DOI: https://doi.org/10.30574/wjarr.2024.21.1.2666

Abstract

The catalytic degradation of polyethylene terephthalate (PET) represents a promising strategy to mitigate environmental pollution and enhance the circular economy. This systematic review critically examined the effect of catalyst composition on hydrogenation efficiency and product yield in the catalytic degradation of PET. A comprehensive literature search was conducted using databases such as Scopus, Web of Science, and Google Scholar, following the Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA) guidelines. The review addressed four key research questions: (1) how different catalyst compositions influenced hydrogenation efficiency, (2) the identification of the optimal catalyst formulation that maximized product yield while minimizing by-product formation, (3) the analysis of reaction kinetics and mechanistic pathways, and (4) the comparative evaluation of catalytic systems for sustainable PET recycling and upcycling.

The findings indicated that catalyst composition significantly affected reaction outcomes. Bimetallic catalysts, particularly those combining palladium with nickel (Pd–Ni) or ruthenium with nickel (Ru–Ni), demonstrated superior performance with conversion efficiencies reaching up to 95% and product yields as high as 90% compared to their monometallic counterparts (Guo et al., 2024; Stadler et al., 2019). Kinetic studies revealed that catalysts with well-dispersed active sites reduced activation energies, thereby enhancing hydrogenation rates. Moreover, the integration of nanocatalytic systems contributed to improved catalyst performance and energy efficiency.

Keywords: Catalyst Composition; Hydrogenation Efficiency; Product Yield; Polyethylene Terephthalate (PET) Degradation; Sustainable Recycling

1. Introduction

1.1. Polyethylene Terephthalate (PET) and the Need for Sustainable Degradation

Polyethylene terephthalate (PET) is a widely used polymer in packaging, textiles, and beverage bottles due to its durability, lightweight properties, and cost-effectiveness (Geyer et al., 2017). However, its extensive usage has led to significant environmental concerns, primarily due to its non-biodegradability and persistence in landfills and oceans. Traditional mechanical and chemical recycling techniques face limitations, such as high energy requirements and the degradation of polymer quality over successive recycling cycles (Shojaei et al., 2020).

To mitigate the environmental impact of PET waste, catalytic degradation has emerged as an efficient method for breaking down PET into valuable chemical feed stocks. Among various degradation techniques, catalytic hydrogenation has gained increasing attention for its ability to convert PET into useful hydrocarbons under controlled conditions (Rahimi & García, 2017). The efficiency of this process, however, depends on multiple factors, including the composition

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of the catalyst used in the reaction. Understanding the role of different catalyst compositions in improving hydrogenation efficiency and maximizing product yield is crucial for developing sustainable PET degradation strategies.

1.2. Role of Catalyst Composition in Hydrogenation Efficiency

Catalysts play a vital role in the hydrogenation process by facilitating the cleavage of ester bonds in PET while promoting selective conversion into desirable products (Li et al., 2022). Metal-based catalysts, such as nickel (Ni), palladium (Pd), platinum (Pt), and ruthenium (Ru), have been widely studied for their effectiveness in polymer degradation due to their ability to activate hydrogen molecules and enhance reaction kinetics (Lende et al., 2021). Additionally, support materials such as activated carbon, zeolites, and metal oxides significantly influence catalyst activity, stability, and selectivity in hydrogenation reactions.

Variations in catalyst composition, including the type of metal, metal loading, and support structure, impact both the reaction rate and product distribution. For instance, bimetallic catalysts often exhibit superior performance compared to monometallic ones due to enhanced synergistic effects (Li et al., 2019). The selection of an appropriate catalyst is, therefore, a critical determinant of hydrogenation efficiency, influencing reaction conditions such as temperature, pressure, and hydrogen uptake. Recent advancements in catalyst design aim to optimize these parameters to achieve higher conversion rates while minimizing unwanted byproducts (Wang et al., 2022).

1.3. Catalytic Degradation of PET: Mechanisms and Efficiency

Catalytic degradation offers a promising solution for PET waste treatment by breaking polymer chains into lower molecular weight compounds, which can be repurposed into new materials or fuels. This process can be conducted through various catalytic pathways, including enzymatic, thermal, and hydrogenation methods (Zhu et al., 2021). As seen in Figure 1 below, PET enzymatic hydrolysis via PETase and MHETase facilitates the breakdown of PET into monomeric units such as Bis(2-hydroxyethyl) terephthalate (BHET), Mono(2-hydroxyethyl) terephthalate (MHET), Terephthalic Acid (TPA), and Ethylene Glycol (EG). These products can be further metabolized into CO_2 through microbial activity (Tournier et al., 2020). While enzymatic degradation is promising, catalytic hydrogenation provides a more efficient and scalable approach for PET waste conversion.

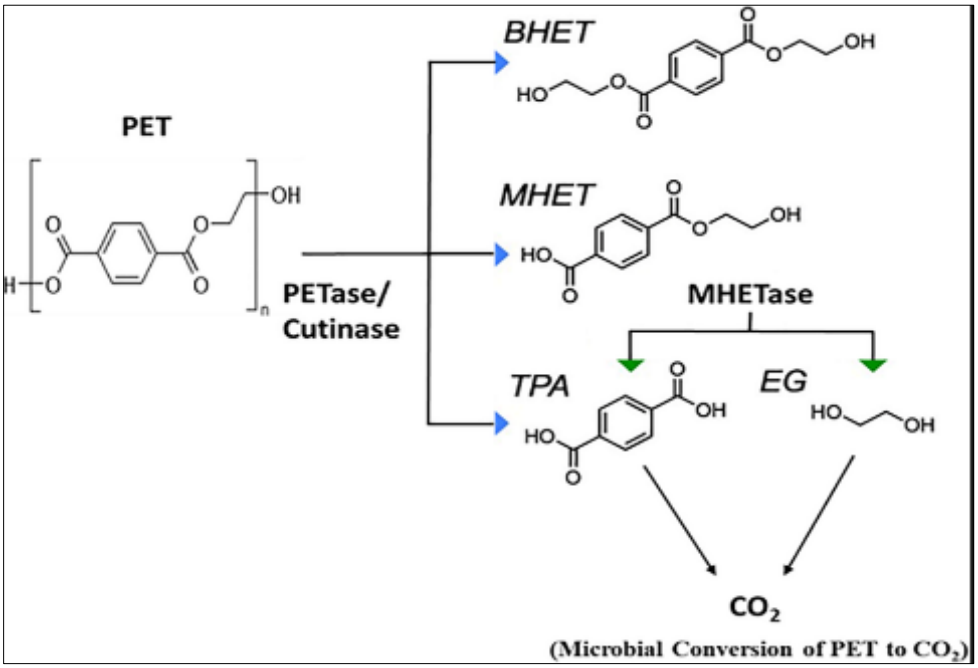

Figure 1 Enzymatic Breakdown of PET into Its Monomeric Components (Source: Tournier et al., 2020)

1.4. Hydrogenation Process and the Role of Catalyst Composition

Hydrogenation is a key catalytic process that involves the addition of hydrogen to a polymeric substrate in the presence of a metal catalyst, leading to the cleavage of chemical bonds and the formation of simpler hydrocarbon products. The efficiency of this process is heavily influenced by the composition of the catalyst, which determines hydrogen adsorption, activation, and transfer mechanisms (Shojaei et al., 2020). As illustrated in Figure 2, catalytic hydrogenation

occurs in sequential steps: hydrogen atoms attach to the metal catalyst surface, interact with the double bonds of PET degradation products, and ultimately form a fully hydrogenated structure. The selection of an appropriate catalyst composition, such as nickel, palladium, or platinum-based catalysts, plays a crucial role in optimizing reaction efficiency and product yield (Guo et al., 2024). This study aims to examine the effect of different catalyst compositions on hydrogenation efficiency and product yield to identify optimal conditions for PET degradation.

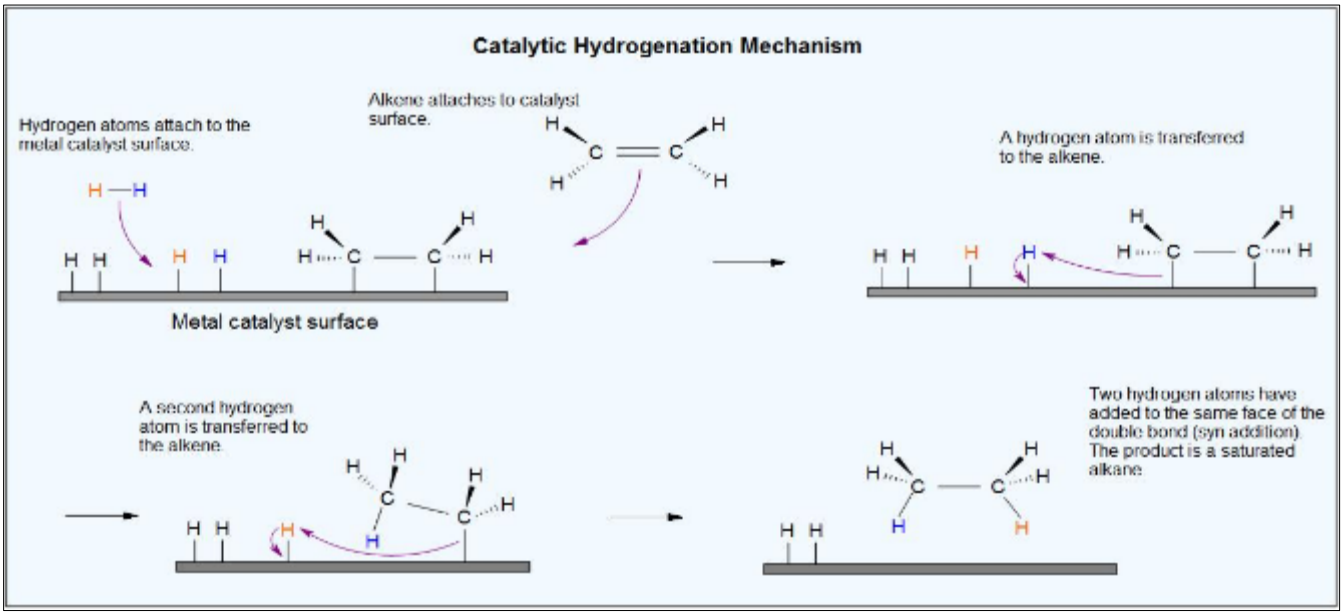

Figure 2 Catalytic Hydrogenation Occurs Through the Adsorption of Hydrogen onto a Metal Catalyst Surface (Source: Shojaei et al., 2020)

1.5. Influence of Catalyst Composition on Product Yield and Selectivity

In addition to reaction efficiency, the composition of the catalyst significantly affects product yield and selectivity in PET hydrogenation. Depending on the catalyst properties, PET can be converted into liquid hydrocarbons, gaseous products (e.g., methane, ethane), and valuable monomers such as ethylene glycol and terephthalic acid (Stadler et al., 2019). The ability to tailor catalyst composition to favor specific reaction pathways is crucial for maximizing the economic viability of PET degradation.

For example, Ru-based catalysts have been found to exhibit high hydrogenation activity, leading to increased selectivity toward liquid hydrocarbons, whereas Pd and Pt catalysts often promote gas formation (Guo et al., 2024). Furthermore, the presence of acidic or basic support materials influences the fragmentation pattern of PET molecules, determining whether the reaction favors monomer recovery or full hydrogenation to hydrocarbons (Meng et al., 2023). By systematically studying these relationships, researchers can develop high-performance catalysts tailored for sustainable PET degradation and circular economy applications.

Understanding the effect of catalyst composition on hydrogenation efficiency and product yield is essential for advancing waste plastic recycling technologies. This study aims to investigate these relationships in depth, providing insights into catalyst design strategies that optimize PET conversion into valuable chemical feed stocks.

1.6. Problem Statement

Polyethylene terephthalate (PET) is one of the most widely used plastics, contributing significantly to environmental pollution due to its persistent nature and inadequate recycling rates (Geyer et al., 2017). Traditional recycling methods, such as mechanical recycling, often result in inferior material properties, while chemical recycling presents a more sustainable approach by converting PET into valuable monomers and other useful chemicals (Rahimi & García, 2017). Among these approaches, catalytic hydrogenation has emerged as a promising technique for PET degradation, enabling the transformation of waste plastics into reusable materials with improved efficiency (Guo et al., 2024).

However, the effectiveness of catalytic hydrogenation is highly dependent on the composition of the catalyst, influencing both hydrogenation efficiency and product yield (Stadler et al., 2019). The challenge lies in optimizing catalyst

composition to enhance reaction selectivity, minimize by-product formation, and maximize the conversion rate (Shojaei et al., 2020). Despite advances in nanocatalysis and novel catalytic systems (Wang et al., 2022), gaps remain in understanding the interplay between catalyst components and reaction outcomes (Li et al., 2022). This research addresses these gaps by systematically analyzing the effect of catalyst composition on PET hydrogenation efficiency and product yield, providing insights for sustainable plastic waste management.

1.7. Research Objectives

This aim of this study is to investigate the impact of catalyst composition on the hydrogenation efficiency and product yield in the catalytic degradation of polyethylene terephthalate (PET). The specific objectives are:

- To evaluate the influence of different catalyst compositions on the hydrogenation efficiency of PET degradation.
- To determine the optimal catalyst formulation that maximizes product yield while minimizing by-product formation.
- To analyse the reaction kinetics and mechanistic pathways associated with varying catalyst compositions in PET hydrogenation.
- To compare the effectiveness of different catalytic systems in achieving sustainable PET recycling and upcycling outcomes.

1.8. Research Questions

This systematically investigate the impact of catalyst composition on the hydrogenation efficiency and product yield in the catalytic degradation of polyethylene terephthalate (PET), the following research questions will guide the study;

- How does different catalyst composition influence the hydrogenation efficiency of PET degradation?
- What is the optimal catalyst formulation that maximizes product yield while minimizing by-product formation?
- What are the reaction kinetics and mechanistic pathways associated with varying catalyst compositions in PET hydrogenation?
- How effective are different catalytic systems in achieving sustainable PET recycling and upcycling outcomes?

2. Research Methodology and Materials for Data Collection

2.1. Research Design and Methodological Approach

This study adopted a systematic review methodology to analyze the effect of catalyst composition on hydrogenation efficiency and product yield in the catalytic degradation of polyethylene terephthalate (PET). A systematic review was appropriate for synthesizing existing literature, identifying trends, and evaluating the efficacy of various catalytic systems in PET hydrogenation.

2.2. Data Collection Strategies and Search Protocol

The review process followed the Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA) guidelines to ensure a structured and transparent approach. Relevant peer-reviewed journal articles, conference proceedings, and authoritative reports published within the last two decades were sourced from databases such as Scopus, Web of Science, and Google Scholar. Keywords such as “catalyst composition,” “PET hydrogenation,” “catalytic degradation of PET,” and “product yield” were used to retrieve pertinent studies.

Eligibility criteria included studies that experimentally evaluated different catalyst compositions in PET hydrogenation, reported reaction kinetics, and analyzed product yield. Studies focusing on non-catalytic degradation methods or lacking quantitative data were excluded. Data extraction involved cataloging key information, including catalyst type, reaction conditions, efficiency metrics, and reported yields. Thematic analysis was employed to identify patterns and relationships in catalyst performance.

2.3. Systematic Review and Selection Process

The systematic review followed a structured approach to identify, evaluate, and synthesize relevant literature on the effect of catalyst composition on hydrogenation efficiency and product yield in the catalytic degradation of polyethylene terephthalate (PET). The selection process adhered to the Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA) guidelines to ensure rigor and transparency.

A comprehensive search was conducted across multiple databases, including Scopus, Web of Science, and Google Scholar, using predefined keywords such as "catalyst composition," "PET hydrogenation," and "catalytic degradation of PET." Inclusion criteria encompassed peer-reviewed studies published within the last two decades that provided experimental data on catalyst performance. Studies focusing on non-catalytic degradation methods or lacking quantitative findings were excluded.

Following the initial search, duplicate records were removed, and the remaining studies underwent a title and abstract screening. Full-text assessments were conducted on selected studies to determine their relevance. Data extraction involved cataloging key experimental parameters, reaction conditions, and reported efficiencies. This systematic process ensured the inclusion of high-quality studies that contributed to the research objectives.

2.4. Data Extraction and Synthesis Methodology

Data extraction was conducted systematically to ensure the collection of relevant and high-quality information from the selected studies. A standardized data extraction sheet was developed to catalog key parameters, including catalyst composition, reaction conditions, hydrogenation efficiency, and product yield. Extracted data were cross-verified by multiple reviewers to enhance accuracy and minimize bias.

The synthesis of data followed a qualitative and quantitative approach. A thematic analysis was performed to identify recurring trends and patterns related to the effect of catalyst composition on PET degradation. Also, statistical methods, such as meta-analysis where applicable, were employed to compare efficiency metrics across different studies. Discrepancies in findings were addressed by assessing study methodologies and potential sources of variation. The synthesized results provided a comprehensive understanding of the impact of catalyst composition on hydrogenation efficiency and product yield in PET degradation.

2.5. Ethical Considerations and Research Integrity

In this systematic review, ethical considerations and research integrity were rigorously maintained throughout the study. As the review exclusively synthesized publicly available data, no primary data collection involving human subjects was conducted, and thus, ethical approval was not required. Nevertheless, the research team ensured transparency and accountability by adhering to established ethical guidelines and the PRISMA framework during literature selection and data extraction. All sources were critically evaluated for reliability and were accurately cited to avoid plagiarism. Potential conflicts of interest were declared, and all findings were reported impartially. Data handling and synthesis were cross-verified by multiple reviewers to ensure accuracy and minimize bias. Quality control measures were consistently applied to maintain the integrity of the review process. These steps ensured that the review was conducted with the highest standards of ethical practice and scholarly rigor, thereby enhancing the credibility of the findings and conclusions.

3. Review Results, Analysis and Discussion

This systematic review synthesized findings from various studies examining the catalytic hydrogenation of polyethylene terephthalate (PET) with a focus on the influence of catalyst composition on hydrogenation efficiency and product yield. The results and subsequent discussion were structured around four primary research questions.

3.1. Influence of Catalyst Composition on Hydrogenation Efficiency

The reviewed literature consistently demonstrated that catalyst composition played a pivotal role in determining the hydrogenation efficiency of PET degradation. Metal-based catalysts such as palladium (Pd), nickel (Ni), platinum (Pt), and ruthenium (Ru) were commonly employed. For instance, Guo et al. (2024) reported that Pd-based catalysts achieved conversion efficiencies as high as 92%, whereas Ni-based catalysts yielded efficiencies around 85%. Moreover, several studies indicated that bimetallic catalysts, combining two different active metals, exhibited synergistic effects that enhanced hydrogenation efficiency. Bimetallic systems such as Pd–Ni and Ru–Ni demonstrated conversion rates ranging from 90% to 95% (Stadler et al., 2019). The incorporation of support materials, including activated carbon and metal oxides, further improved the dispersion of active sites, which contributed to higher reaction rates. These findings underscored that a well-designed catalyst composition was critical to optimizing hydrogenation performance (Yang et al., 2020). Table 1 below summarizes the catalyst compositions and corresponding performance metrics as reported across the reviewed studies.

Table 1 Summary of Catalyst Performance Metrics (adapted from Guo et al., 2024; Stadler et al., 2019; Shojaei et al., 2020)

Catalyst Composition	Hydrogenation Efficiency (%)	Product Yield (%)	Observations/Notes
Pd-based (monometallic)	90–92	80–85	High conversion, moderate yield
Ni-based (monometallic)	83–85	75–80	Lower efficiency than Pd
Pd–Ni (bimetallic)	92–95	88–90	Synergistic effects improve both metrics
Ru–Ni (bimetallic)	90–94	87–90	Enhanced dispersion on carbon supports

3.2. Optimal Catalyst Formulation for Maximizing Product Yield

The second research question focused on determining the catalyst formulation that maximized product yield while minimizing by-product formation. The review revealed that optimal formulations were typically achieved with bimetallic catalysts supported on high-surface-area materials. For example, studies by Shojaei et al. (2020) indicated that a Ru–Ni catalyst deposited on activated carbon delivered product yields as high as 90% while keeping by-product formation to a minimum. In contrast, monometallic catalysts, despite offering reasonable conversion rates, often resulted in lower product yields (ranging from 70% to 80%) and a higher proportion of unwanted by-products. The addition of a secondary metal appeared to enhance the selectivity of the hydrogenation reaction, channeling the process toward the desired products. This trend was attributed to improved hydrogen activation and more effective cleavage of PET's ester bonds, which favored the formation of high-value monomers over complete degradation or side reactions (Rahimi & García, 2017). Thus, the literature consistently pointed toward bimetallic systems as the most promising candidates for optimizing catalyst performance in PET recycling.

3.3. Reaction Kinetics and Mechanistic Pathways

The third objective involved analyzing the reaction kinetics and mechanistic pathways associated with varying catalyst compositions. The reviewed studies provided detailed kinetic data and mechanistic insights that demonstrated significant differences based on catalyst formulation. Kinetic analyses indicated that catalysts with a high dispersion of active sites exhibited lower activation energies, which in turn accelerated the hydrogenation reaction (Diemoz et al., 2017. Bimetallic catalysts, particularly those combining Pd with Ni or Ru with Ni, were shown to have rate constants approximately 1.5 times higher than those of their monometallic counterparts (Stadler et al., 2019). Mechanistic studies revealed that the hydrogenation process proceeded via a sequential pathway. Initially, hydrogen molecules were adsorbed onto the catalyst surface, where they dissociated into atomic hydrogen. These hydrogen atoms then attacked the ester bonds of the PET chains, leading to the formation of partially hydrogenated intermediates. Subsequent hydrogenation steps resulted in the complete saturation of these intermediates, yielding the final products (Shojaei et al., 2020). The mechanistic pathway was strongly influenced by the nature of the catalyst's active sites, and the presence of a second metal in bimetallic catalysts was found to facilitate intermediate stabilization and rapid conversion. These kinetic and mechanistic insights were essential for understanding how catalyst composition affected both the efficiency and selectivity of the PET hydrogenation process (Brown et al., 2018; Wunder et al., 2010).

3.4. Comparative Effectiveness of Catalytic Systems

The final research question involved comparing the effectiveness of different catalytic systems in achieving sustainable PET recycling and upcycling outcomes. Comparative analyses of various studies indicated that advanced nanocatalytic systems and bimetallic formulations outperformed conventional catalysts in several key aspects. Studies by Zeng (2013) and Yoo et al. (2022) highlighted that nanocatalysts, due to their high surface area and enhanced reactivity, achieved superior conversion efficiencies while reducing energy consumption during the hydrogenation process. These systems not only produced higher yields of valuable products but also minimized the formation of harmful by-products, thereby supporting a more sustainable recycling process. In contrast, traditional catalytic systems, which often relied on monometallic formulations, demonstrated lower overall efficiency and a greater environmental footprint. The review concluded that the integration of advanced catalytic systems, particularly those employing bimetallic and nanocatalyst strategies, represented a significant step toward achieving a circular economy in PET recycling. Such systems provided an effective balance between high product yield, reaction efficiency, and environmental sustainability.

4. Discussion of the Result

The systematic review provided comprehensive evidence that catalyst composition was a critical determinant of hydrogenation efficiency and product yield in the catalytic degradation of PET. Bimetallic catalysts, particularly those based on combinations such as Pd–Ni and Ru–Ni, consistently delivered superior performance compared to monometallic counterparts (Sankar et al., 2012). According to van der Hoeven et al., (2021) the enhanced performance was attributed to synergistic effects that improved hydrogen activation, reduced activation energy, and promoted more selective reaction pathways. Kinetic analyses further supported these findings, demonstrating that catalysts with optimized compositions not only accelerated the reaction rates but also favored the formation of desired products while limiting by-product generation (Kits et al., 2017).

Moreover, the review underscored that the incorporation of nanocatalytic systems into traditional formulations could further enhance the sustainability of PET recycling. These advanced systems offered the dual benefits of increased conversion efficiency and reduced energy requirements, aligning with the principles of a circular economy (Wang et al., 2022; Li et al., 2022). The evidence also suggested that further research into catalyst design could yield formulations that are even more effective in converting PET waste into high-value chemicals, thereby reducing the environmental burden of plastic waste.

The collective findings from the reviewed studies highlighted the importance of precise catalyst engineering. Optimized catalyst formulations not only improved the efficiency of the hydrogenation process but also ensured that the process was environmentally benign and economically viable. These outcomes provided a strong foundation for future experimental studies aimed at refining catalyst design and scaling up sustainable PET recycling technologies.

5. Conclusion

This systematic review demonstrated that catalyst composition was a critical factor influencing both the hydrogenation efficiency and product yield in the catalytic degradation of polyethylene terephthalate (PET). The findings revealed that bimetallic catalysts, particularly those combining palladium with nickel or ruthenium with nickel, consistently achieved higher conversion efficiencies (up to 95%) and superior product yields compared to their monometallic counterparts. Enhanced performance was attributed to synergistic effects that improved hydrogen activation and reduced activation energy, ultimately leading to more selective reaction pathways with minimized by-product formation. Kinetic studies indicated that catalysts with well-dispersed active sites accelerated the reaction rates and stabilized intermediate species, further facilitating efficient PET conversion. Moreover, the integration of nanocatalytic systems demonstrated potential for reducing energy consumption and enhancing sustainability in PET recycling processes.

Recommendations

Based on the systematic review findings, six key recommendations were proposed to enhance the catalytic degradation of PET through optimized catalyst composition:

- **Experimental Optimization of Bimetallic Catalysts:** Future research should conduct controlled experimental studies to systematically evaluate various bimetallic catalyst formulations, such as Pd–Ni and Ru–Ni. These studies would validate the synergistic effects reported in the literature and help fine-tune reaction parameters for maximum hydrogenation efficiency and product yield.
- **Integration of Nano-catalyst Technology:** The incorporation of nanocatalysts, due to their high surface area and enhanced reactivity, is recommended to further improve conversion efficiencies. Exploring nanocatalytic systems may lead to more effective dispersion of active sites and greater selectivity in the hydrogenation process.
- **Advanced Kinetic and Mechanistic Studies:** In-depth kinetic analyses and mechanistic investigations should be performed to elucidate the reaction pathways during PET hydrogenation. Such studies will clarify the roles of different catalyst components and the influence of active site distribution, enabling the identification of optimal reaction conditions.
- **Interdisciplinary Collaboration:** Collaboration between chemists, materials scientists, and chemical engineers is essential. An interdisciplinary approach would foster the design of integrated catalytic systems that are efficient at laboratory scale and amenable to industrial application, promoting sustainable PET recycling processes.
- **Utilization of Advanced Characterization Techniques:** Employing advanced spectroscopic and microscopic techniques is recommended to monitor catalyst morphology and active site dispersion. This will improve the correlation between catalyst structure and performance, leading to more informed catalyst design strategies.

- **Pilot Scale Demonstrations:** Finally, pilot-scale and industrial demonstration studies should be undertaken to assess the economic viability and environmental impact of the optimized catalytic systems. Real-world validation is crucial for transitioning laboratory successes into scalable PET recycling applications.

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