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Keywords: Power-to-X; Machine Learning; Power-to-Gas; Power-to-Liquid; Power-to-Heat; Data-Driven Optimization; Energy Storage; Green Hydrogen; Green Ammonia; Sustainable Aviation Fuel

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Review

Recent Advancements in Applying Machine Learning in Power-to-X Processes: A Literature Review

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Abstract: For decades, fossil fuels have been the backbone of reliable energy systems, offering unmatched energy density and flexibility. However, as the world shifts toward renewable energy, overcoming the limitations of intermittent power sources requires a bold reimagining of energy storage and integration. Power-to-X (PtX) technologies, which convert excess renewable electricity into storable energy carriers, offer a promising solution for long-term energy storage and sector coupling. Recent advancements in machine learning (ML) have revolutionized PtX systems by enhancing efficiency, scalability, and sustainability. This review provides a detailed analysis of how ML techniques, such as deep reinforcement learning, data-driven optimization, and predictive diagnostics, are driving innovation in Power-to-Gas, Power-to-Liquid, and Power-to-Heat systems. While ML applications have shown great potential in optimizing operational decisions and managing uncertainties in renewable energy integration, challenges such as data quality, real-time processing, and scalability remain. Addressing these gaps presents important future research opportunities. These advancements are critical to decarbonizing hard-to-electrify sectors such as heavy industry, transportation, and aviation, aligning with global sustainability goals.

Keywords: power-to-X; machine learning; power-to-gas; power-to-liquid; power-to-heat; data-driven optimization; energy storage; green hydrogen; green ammonia; sustainable aviation fuel

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1. Introduction

The global energy landscape is transforming, shifting from reliance on fossil fuels to an increased adoption of renewable energy sources. While essential for sustainability, this transition introduces challenges, particularly concerning the intermittent nature of renewable energy sources such as wind and solar power. Historically, fossil fuels have offered unparalleled reliability and adaptability in meeting the energy demands of various sectors thanks to their high degree of accessibility, flexibility, portability [1,2] and storability with high density of energy. As shown in Figure 1, fossil fuels have dominated global energy generation for decades, but clean energy sources have steadily increased their share over recent years. However, this progress is still insufficient to fully offset the dependency on fossil fuels.

Fossil fuels have adeptly managed fluctuations in supply and demand, ensuring a balance within the energy systems. However, the variability in renewable energy production necessitates robust solutions to ensure stability in the energy supply, aligning generation with demand across various timescales. The intermittent generation from renewables, characterised by fluctuations ranging from seconds to seasons, presents a significant barrier to their broader implementation. Energy storage systems (ESS) can play a crucial role in mitigating these fluctuations and achieving a more reliable and consistent energy supply. ESSs help store excess energy generated from renewable sources during times of surplus production, making it available when demand is higher or production is low [3,4]. By smoothing out these supply-demand mismatches, ESSs not only enhance grid stability but also facilitates the integration of renewables into the existing energy infrastructure.

This adaptability is crucial for driving the transition toward cleaner energy systems without compromising reliability.

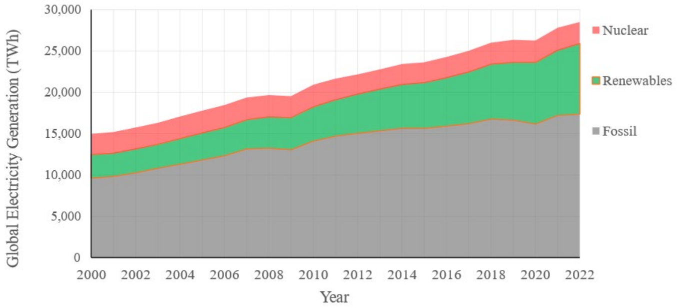


Figure 1. Annual electricity generation data 2000-2022 [5].

Although there are advancements in energy storage like batteries designed for short-term balancing, the limitations of these solutions become apparent when considering longer-duration storage, as evidenced by their low energy densities and high costs compared to liquid fuels like diesel, gasoline, or liquid methane [6–8]. Also, the geographic disparity between renewable energy sources and major consumption centres further complicates direct electrification efforts.

These challenges underscore the necessity for innovative approaches like Power-to-X (PtX) technologies. While battery systems store electricity directly, PtX extends this by converting energy into other forms like hydrogen or synthetic fuels, enabling longer-term storage and versatility across different sectors. Together, they provide a comprehensive solution for both short- and long-term energy storage challenges. It is projected that by 2050, PtX and cogeneration will form the foundation of a resilient, decentralised, and carbon-neutral energy system in Europe [9]. This transformation will empower industries and citizens across the continent to generate clean heat and energy locally, in a manner that is reliable, cost-effective, and efficient.

The development of PtX systems faces a range of challenges across economic, technical, environmental, regulatory, and infrastructural areas. Overcoming these challenges requires collaboration and innovation in various fields, including technological advancements, regulatory adjustments, market growth, and improved modelling approaches [4,10–12]. ML plays a crucial role in tackling these issues, particularly as PtX systems become more complex with the integration of renewable energy sources. ML provides effective solutions by simplifying complex optimisation tasks, improving predictive and forecasting capabilities, real-time decision-making [13], high-throughput screening and clustering, and simulation acceleration.

While the existing review studies have examined the application of ML in each PtX-related technology area, per se, the literature lacks a holistic overview on how ML can evolve the development of the entire PtX system. Several review studies are found in the literature that have a focus on specific components of PtX and PtX-related systems; for instance, some researchers have provide comprehensive review studies of proton exchange membrane (PEM) electrolysers, with a particular focus on the integration of ML, to enhance control-oriented modelling, dynamic operation, and control strategies aimed at enhancing system stability and efficiency [14–17]. Also, Iqbal et al. (2024) [18] conducted an in-depth bibliometric analysis of ML in optimising hydrogen production through electrochemical methods. Some other have explored recent advancements in environmental, economic, and policy considerations in hydrogen production technologies and the role of ML and data-driven methods [19–21].

Very few review studies are found in the literature that have a particular focus on PtX systems (as a whole) and ML, such as the work by Ullah et al. (2022) [22] which explored the integration of advanced data-driven methodologies like IoT, big data analytics, and ML to optimise PtX operations. They highlight the potential of these technologies to improve sustainability and efficiency by dynamically adjusting operational parameters to manage renewable energy intermittency. They suggest that challenges such as data management, computational demands, and the need for real-time optimisation persist. While their work is comprehensive, it lacks sufficient depth in ML applications. Another contribution to this area is the work by Birkner (2017) [23], which, while not a review paper and not recent, discusses the application of big data tools and neuronal networks in smart energy systems, including PtX technologies. The study highlights the role of ML-driven predictive tools in optimising PtX operations, particularly in balancing energy generation and improving grid stability.

A review of the existing studies shows that, although considerable research has been conducted on specific components of PtX-related technologies, there remains a notable gap in reviewing works that focus directly on PtX systems as a whole, incorporating explicit references to any member of the PtX family—such as Power-to-Gas, Power-to-Liquid, Power-to-Ammonia, and etc—in combination with ML and data-driven methods. On the other hand, researchers rarely have studied the broad topic of PtX without focusing on a specific type, but the study by Kim et al. (2023) [24] is worth mentioning, where researchers developed a data-driven, reliability-based optimization approach using generative adversarial networks (GANs) to manage renewable uncertainty across grid-assisted PtX systems. This review aims to address that gap by focusing exclusively on studies where the PtX concept, in any of its forms, is paired with machine learning. Table A1 provided in the Appendix A, encompasses recent review papers that has explored specific subjects that can be related to PtX systems, such as green hydrogen production technologies, catalysts, materials, etc.

The present review provides a comprehensive analysis of the role of ML in different types of PtX systems, including Power-to-Gas, Power-to-Liquid, and Power-to-Heat. While the two above-mentioned works deliver a very general overview on data-driven methods for operational optimisation of PtX systems, and take a broader view in sustainable energy practices, the current work distinguishes itself by covering recent advances achieved by ML in different specific types of PtX systems, including technological innovation, optimisation, system integration, forecasting, prediction, and strategic environmental and economic analysis.

The overall structure of the article begins with an introduction that briefly outlines the significance of the transition to renewable energy, PtX systems, and the challenges involved. This is followed by a review of the methodology used to identify and classify the literature. The main body of the review then introduces the concepts and challenges of PtX systems, providing necessary background, followed by an exploration of ML concepts and their evolution. The heart of the review is dedicated to examining ML applications in PtX through four key categories that map onto main different types of PtX, as outlined in the methodology section. These categories are:

1. Machine Learning & Power-to-Gas Systems
2. Machine Learning & Power-to-Liquid Systems
3. Advances in Sustainable Combustion and Fuel Optimisation for Next-Generation Engines
4. Machine Learning & Power-to-Heat

Finally, the article concludes by synthesizing the findings and highlighting future research directions.

2. Review Methodology

In the context of applying ML to PtX processes, most research has focused on reviewing specific aspects of PtX in isolation. This body of work mostly encompasses process and technology optimisation in Multi-Energy and Integrated Renewable Energy systems (IRESs) and power networks.

An organized search strategy was employed to explore the relevant literature, utilizing approximately 140 keywords in specifically designed logical queries on Scopus. The search was conducted in stages, systematically covering different categories of studies and discovering the overlaps. This approach aimed to investigate the application of machine learning methods in the context of Power-to-X and related areas, which has emerged as a young but growing research area since almost 2008. A total of 507 peer-reviewed journal articles and review papers published between 2008 and 2024 were identified. Figure 2 illustrates the increasing research interest in this field since 2008. Notably, the total number of studies related to PtX, irrespective of machine learning applications, exceeds 50,000 papers. However, machine learning and related keywords were found in only 1.0% of these studies' title, abstract, and keywords.

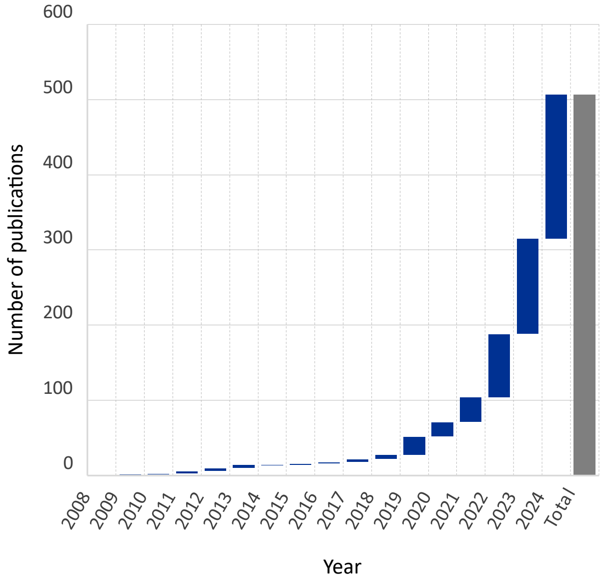
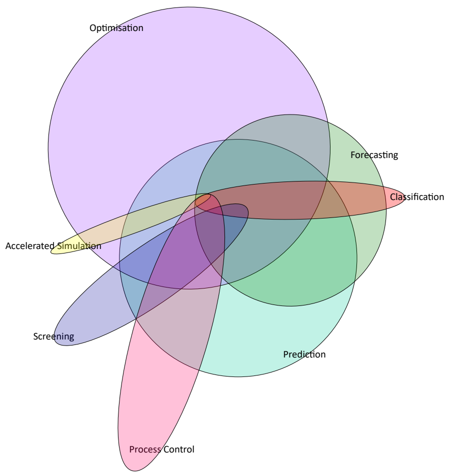


Figure 2. Application of ML in the fields related to PtX process publication trend from Scopus academic search platform.

As part of the data gathering process, and to obtain insightful information, the identified literature was categorized into seven groups based on the primary tasks of machine learning: prediction, forecasting, classification, screening, optimisation, process control, and simulation acceleration. In addition to the frequent interchangeable use of some of these terms –such as prediction and forecasting – in the literature, overlaps exist among them due to the dynamic and innovative nature of machine learning methods and their diverse applications. An analysis of the frequency of different machine learning tasks in the PtX field, along with the overlaps, provides valuable insights (see the Venn diagram in Figure 3a). However, in a number of 61 articles from this collection (mostly review papers), no specific ML-based task or method were mentioned in the title, abstract, and keywords area, and therefore, not being categorised under any of these classes.



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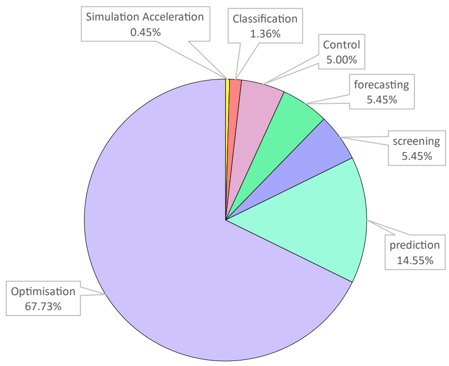

(**b**)

Figure 3. (a) Distribution and overlap of machine learning tasks applied in the field of PtX and sustainable energy systems according to the literature (2016 – 2024). The Venn diagram illustrates the dominant machine learning tasks (optimisation, prediction, and forecasting) and highlights the significant overlap between these categories, as well as their relation to other tasks such as process control, classification, screening, and simulation acceleration; **(b)** Distribution of unique machine

learning tasks in PtX and sustainable energy systems. The pie chart displays the relative frequency of each machine learning task considering only papers that focus exclusively on a single task without overlap with other categories.

As shown in Figure 3a, optimisation, prediction, and forecasting constitute the majority of machine learning applications in PtX research, with significant overlap between these categories. Process control, classification, screening, and simulation acceleration are also applied, though to a lesser extent. It is important to note that the vast majority of studies in the field fall under optimisation, prediction, and forecasting. Figure 3b presents a pie chart comparing the frequency of each machine learning task, focusing on unique studies not shared between other categories.

Given the expansive scope of research in this field, this paper will focus on articles and reviews published in peer-reviewed journals after 2020. After applying manual further screening and eligibility criteria over the 507 papers, a total number of 127 papers were identified to include any keywords directly associated with a type of PtX system. Finally, 53 papers were selected as the most relevant for detailed review, and included in the reviewing process, using Mendeley Software. Besides these included studies, several other references are cited in this study for their contribution to more general subjects related to sustainable development of energy, PtX, and Machine Learning.

Categorising studies in a review can be helpful as it enhances clarity, organisation, and depth, helps identify research gaps, facilitates comparative analysis, and makes the review more accessible and useful for a diverse audience. For the current review, it was done by exploring each study based on specific key questions on

- What is main focus area of the study?
- What specific ML techniques are used?
- What application is ML used for?
- What are the main outcomes of the study?

Addressing these questions for each of the included papers, would also serve as a critical step to understanding the actual contribution of each study to the literature, through a critical perspective. Figure 4 represents the workflow of this review.

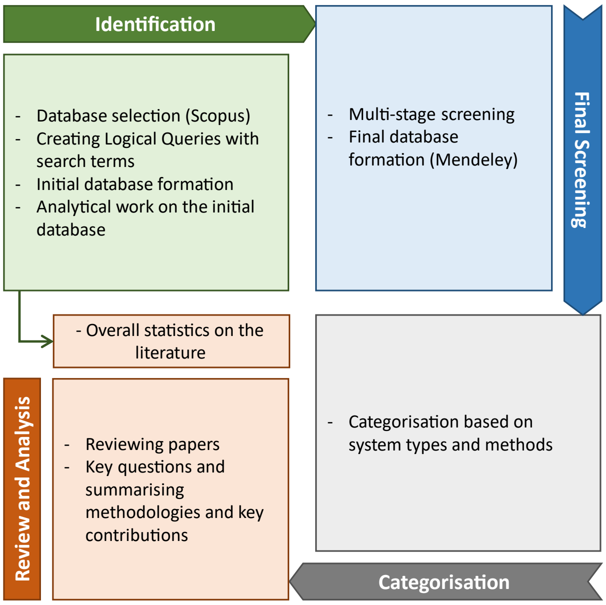

Figure 4. The strategy for identifying and reviewing related literature.

3. Power-to-X Systems: Concepts and Challenges

Power-to-X refers to a suite of technologies that convert electrical power, primarily from renewable sources, into different forms of energy carriers or chemical products. This transformation process aims to overcome the limitations of direct electrification and energy storage by enabling the versatile use of renewable energy across various sectors. The 'X' in PtX (or P2X) stands for various

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end products such as hydrogen (mostly known as P2H2 in the literature), gas (PtG or P2G) – a gaseous energy carrier such as synthetic natural gas, methanol (PtM or P2M), ammonia (PtA or P2A), and other chemicals or fuels (see Figure 5), offering a bridge between renewable energy sources and their broader application in industry, transportation, and beyond. By harnessing excess renewable electricity for the production of these carriers, PtX technologies can play a key role in enhancing energy storage, diversifying energy applications, and facilitating the decarbonisation of sectors traditionally reliant on fossil fuels [5,69]. The flexibility of PtX systems makes them essential for achieving long-term energy sustainability, particularly as global energy demand shifts toward cleaner, more resilient sources.

The concept of PtX is central to addressing the challenges of integrating renewable energy into our current energy systems. It can provide energy storage, transport, and utilisation in forms compatible with existing infrastructure and technologies [70]. Power-to-Hydrogen, where produced electricity is converted to hydrogen through water electrolysis, is identified as the lynchpin of PtX, a foundational step towards the production of sustainable fuels and chemicals that can be used across various sectors, including those that are difficult to decarbonise such as the industrial sector, heavy transportation, and aviation. The production of hydrogen via electrolysis, utilising surplus renewable electricity, facilitates the creation of a flexible and responsive energy system capable of accommodating the inherent unpredictability of wind and solar power [71]. Beyond hydrogen, PtX technologies open the door to a broader spectrum of synthetic fuels, such as methanol and ammonia, which not only provide sustainable alternatives but also leverage existing infrastructure and offer practical solutions for deeply entrenched, hard-to-electrify sectors.

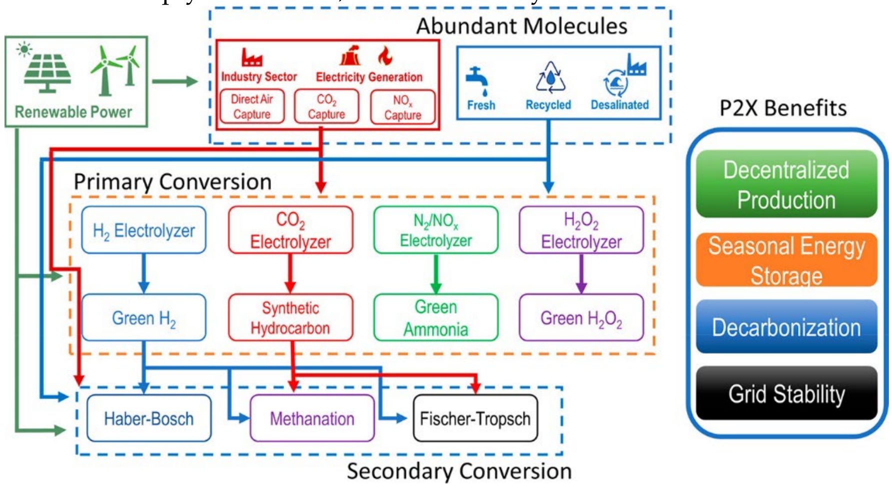

Figure 5. Schematics of power-to-X infrastructure reprinted with permission from [10]. PtX systems primarily begin with electrolysis, where renewable electricity is used to split water into hydrogen and oxygen. This renewable hydrogen can then be applied in secondary processes such as methanation, hydrogenation, and Fischer-Tropsch synthesis to produce hydrocarbon products or ammonia through the Haber-Bosch process, offering a flexible range of outputs. However, additional pathways may also exist depending on the specific PtX technology used.

Furthermore, the integration of PtX technologies leverages existing natural gas grids and equipment. This integration provides a solution for storing and transporting energy and contributes to the decarbonisation of various sectors by providing cleaner alternatives to fossil fuels. PtM and PtA exemplify the potential of PtX to utilise carbon dioxide and nitrogen from the air, turning them into valuable commodities while enhancing the energy system's flexibility and resilience [4,25–27]. As renewable energy scales up, particularly in sectors where direct electrification may not be viable, synthetic fuels emerge as a bridge, enabling the use of established technologies like Internal Combustion Engines (ICEs) in a more sustainable manner.

Contrary to the perception that the future of transportation and energy is exclusively electric, Internal Combustion Engine (ICE) technology continues to evolve, presenting a compatible pathway for utilising synthetic fuels produced via PtX processes. The continuous improvement of the alreadymature technology of ICEs, coupled with the strategic incorporation of PtX-derived fuels, also called as E-fuels, can facilitate a more inclusive and pragmatic approach towards achieving sustainability in transportation and beyond. This perspective does not discount the potential of electric vehicles but rather highlights the diversity of solutions required to address the complex challenges of the global energy transition [28,29]. As we consider these alternatives, E-fuels stand out as a promising solution. Not only are they capable of powering existing ICEs, but they also offer a carbon-neutral pathway by reintroducing captured carbon into the energy cycle.

E-fuels are carbon-neutral and renewable because the carbon they contain is sourced directly from the atmosphere, while the chemical energy stored in them comes from renewable resources like wind or solar power. This process effectively closes the carbon loop, as the CO_2 released during combustion is equal to the amount initially captured. In one sense, it can be viewed as reversing the combustion process by using renewable energy to create fuel, thus reintroducing captured carbon into the energy cycle (see Figure 6).

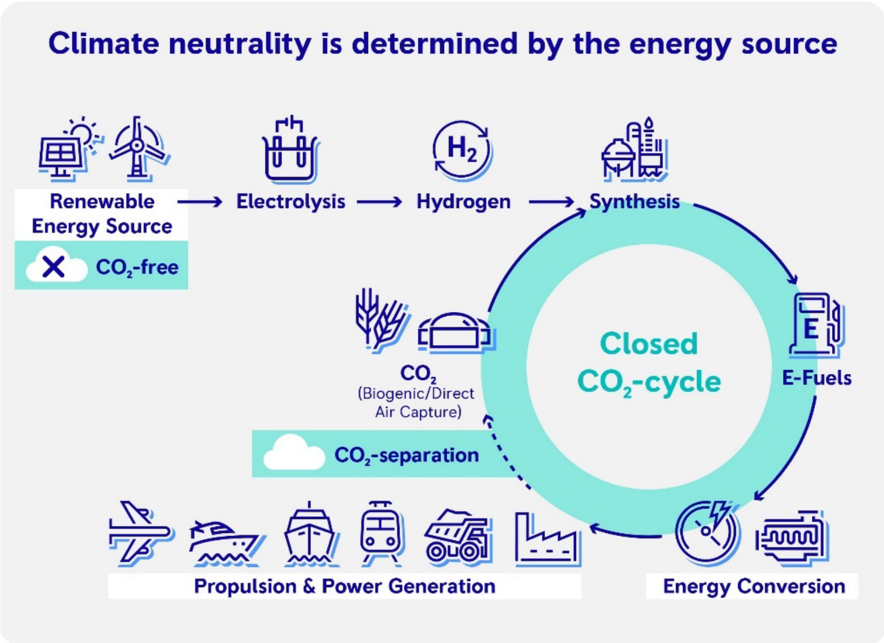

Figure 6. The carbon-neutral cycle of E-fuels, where CO_2 captured from the atmosphere is reused to create fuel using renewable energy, closing the carbon loop. Image credit: MTU-Solutions [30].

The development and implementation of PtX technologies represent a critical juncture in the global effort to transition from fossil fuels to a more sustainable, flexible, and resilient energy system. By leveraging the synergy between renewable energy sources, energy storage technologies, and PtX processes, we can overcome the challenges of intermittency and geographical limitations, paving the way for a decarbonised future that still benefits from the proven capabilities of the current infrastructure and well-established technologies like ICEs.

3.1. What Key Challenges Impede PtX Systems' Progress?

The progression of PtX systems is impeded by multifaceted challenges that span economic, technical, environmental, regulatory, and infrastructural domains. A quick review over these challenges is presented in Figure 7. The economic barriers are particularly pronounced, with high capital and operational costs, especially in the absence of sufficient government incentives. These economic challenges are exacerbated by the high costs associated with renewable electricity and hydrogen storage [4,10–12].

Technically, the maturity of PtX technologies varies, with some systems, like solid oxide electrolyser cells (SOECs), still in the early stages of development [31]. In addition, the technical scalability of PtX technologies is hampered by the limited availability of critical raw materials, such

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as platinum group metals, which are essential for electrolysis processes [12]. The integration of these technologies into existing infrastructures is complex, particularly when coupled with the fluctuating nature of renewable energy sources, which demand dynamic flexibility that many current systems cannot adequately provide [32,33]. This challenge is compounded by the issues of thermal instability and catalyst degradation that arise when operating PtX processes dynamically to match the fluctuating supply of renewable energy, which can complicate the maintenance of consistent product quality [34]. Additionally, the effective utilisation of by-products and waste heat, a potential efficiency booster, remains underexplored, further limiting the overall effectiveness of PtX systems [11].

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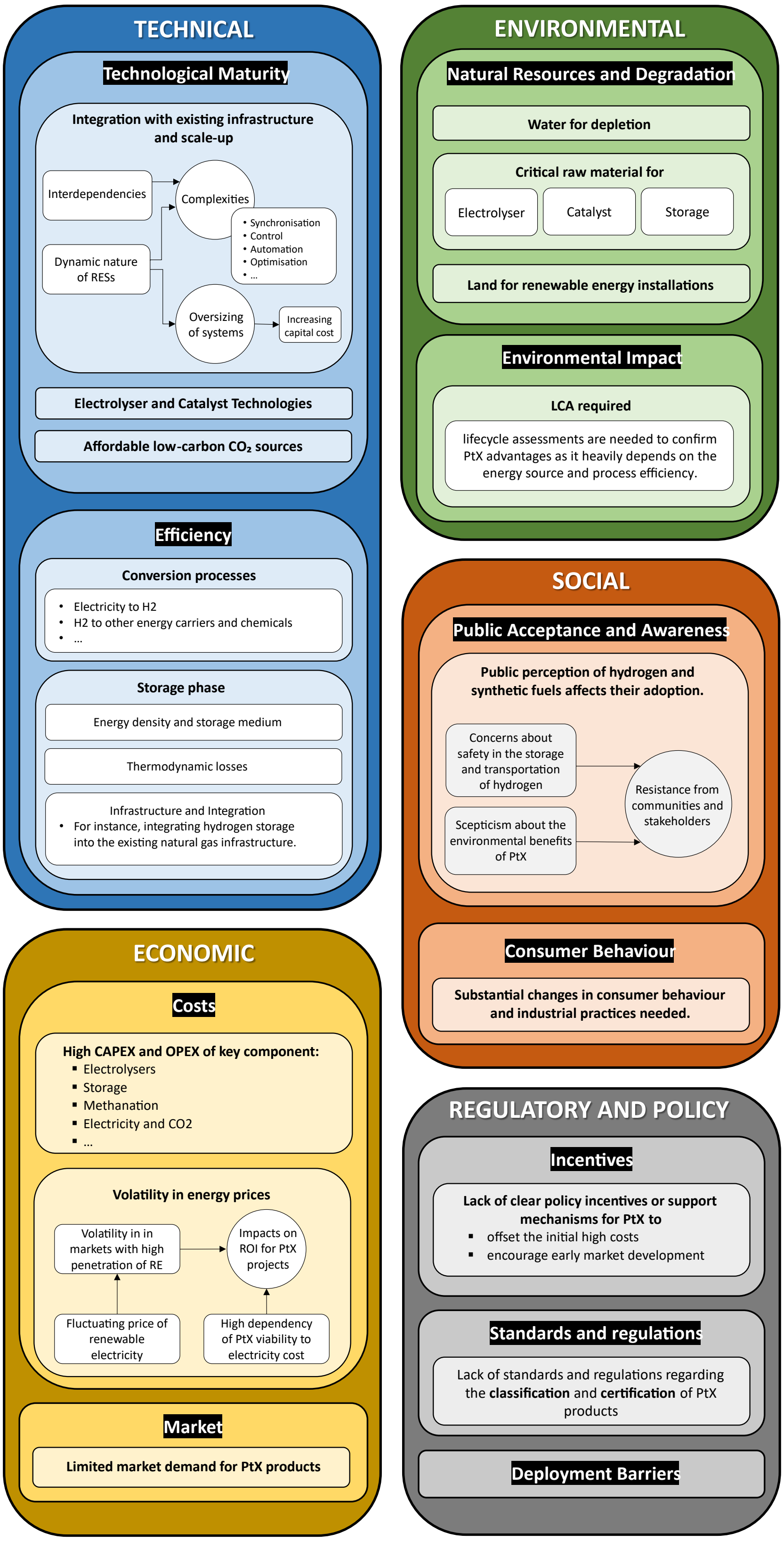

Figure 7. Existing challenges in developing PtX systems.

Environmental challenges also pose significant barriers, particularly in the sourcing and storage of CO_2 and the environmental impact of electrolyser operations, which raise concerns about water depletion and other forms of degradation. Furthermore, the substantial water demand for hydrogen production via electrolysis, though currently considered manageable in some regions, must be carefully monitored as PtX scales up globally [12]. Moreover, the lack of widely adopted sustainability metrics and comprehensive environmental assessments hampers a full understanding of the implications of PtX technologies, particularly within hybrid renewable energy systems (HRES) [31,35]. Lifecycle assessments are needed to confirm PtX advantages as it heavily depends on the energy source and process efficiency.

Regulatory constraints, such as strict standards for natural gas and hydrogen blending, further limit the integration of PtX products into existing energy networks [11]. The lack of a cohesive, application-neutral regulatory framework for PtX technologies presents a significant barrier to their deployment and scaling. Regulatory gaps and the absence of supportive niche markets complicate the commercialisation of PtX systems [36]. The market for PtX products is still developing, and the reliance on public funding shows the current lack of economic viability, and the need for greater market acceptance and infrastructure development to support the widespread commercialisation of PtX systems.

Infrastructural challenges, including geographical variability and the scalability of PtX projects, complicate the large-scale deployment of these technologies. Furthermore, implementing PtX processes in remote locations with high renewable energy potential but limited infrastructure adds to the operational challenges, leading to increased costs and complexity [34]. The transition to decentralised energy systems introduces additional complexities in ensuring stability and security, which are critical for the sustainable operation of PtX technologies [11,31].

Limitations in current modelling and optimisation approaches often lead to oversimplifications that fail to capture the real-world complexities of PtX systems. The need for multi-objective optimisation that considers not only economic factors but also environmental and operational safety metrics is crucial for accurately assessing and improving the performance of these technologies [11]. Without addressing these diverse factors, the potential for PtX systems to meaningfully contribute to decarbonisation efforts may be hindered.

Addressing these intertwined challenges requires a concerted and innovative effort across multiple sectors, including technological innovation, regulatory reform, market development, and enhanced modelling techniques. ML can be a critical enabler in addressing the multifaceted challenges of integrating PtX technologies into existing energy systems. As PtX systems grow in complexity, particularly with the integration of renewable energy sources, ML offers robust solutions by converting complex optimisation tasks into manageable processes, enhancing predictive accuracy and real-time decision-making [13]. Its ability to integrate diverse data sources and optimise energy storage is indispensable for maintaining system stability and efficiency in increasingly decentralised and cyber-physical energy networks [37].

4. ML: Concepts, Evolution, and Impact

ML is a pivotal branch of artificial intelligence (AI) that focuses on enabling computer systems to learn from data, identify patterns, and make decisions with minimal human intervention. Unlike traditional programming, where specific instructions are coded, ML algorithms develop their own logic based on input data, allowing them to adapt and improve over time [38]. ML can be understood as the scientific study of mathematical algorithms and models designed to generate complex rules based on data, thereby automating tasks that would otherwise require human intelligence. These algorithms are categorised by learning styles—such as supervised, unsupervised, and reinforcement learning—and by their function, including classification, regression, and clustering. Deep learning, a subset of ML, specifically focuses on learning data representations through multiple layers of processing, further expanding the capabilities of ML [39]. As ML algorithms have become more advanced, they have revolutionised various industries by solving complex problems and driving innovation, making ML indispensable in the modern technological landscape [40]. The versatility of ML algorithms, combined with their capacity for continuous learning and optimisation, have proven their critical role in advancing technology [41].

The essential elements of ML include representation, which refers to the set of classifiers or the language that a computer system understands to interpret data; evaluation, which involves assessing

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the model's accuracy and effectiveness in making predictions or classifications; and optimisation, the process of improving the model's performance by finding the best parameters or methods that yield the highest evaluation scores. These components are crucial for enabling ML algorithms to learn from data, make predictions, and adapt over time without explicit programming [38,39].

ML is broadly categorised into three main types: supervised learning, unsupervised learning, and reinforcement learning. Supervised learning involves training algorithms on labelled datasets, enabling them to predict outcomes or classify data based on known input-output pairs [39]. This approach is widely used in industries like automotive manufacturing for predictive maintenance, where algorithms can forecast component failures by analysing historical data [41]. Unsupervised learning, on the other hand, deals with unlabelled data, using techniques like clustering and dimensionality reduction to identify hidden patterns or group similar items, which is particularly useful in quality control and process [38,39] through trial and error, making it ideal for optimising complex processes in dynamic environments such as manufacturing and supply chain logistics [40,41]. These types of ML, along with deep learning, a subset focused on learning data representations through multiple layers, are integral to advancing automation, efficiency, and innovation in various technological and industrial domains [39].

The evolution of ML has profoundly impacted industries, particularly within the framework of Industry 4.0, where it has become essential for optimising processes, enhancing automation, and enabling data-driven decision-making. Initially, the integration of ML faced challenges such as data scarcity and technological limitations, but advancements in deep learning and other algorithms have gradually overcome these barriers, leading to widespread industrial applications. ML now plays a crucial role in sectors like smart manufacturing and petrochemicals, where it drives real-time process optimisation, predictive maintenance, and energy efficiency improvements. As research continues to advance, ML is poised to further revolutionise industries by addressing challenges related to data quality and scalability, solidifying its role as a key driver of innovation and efficiency in the modern industrial landscape [40–43]. As these technologies mature, industries are increasingly leveraging ML not just for operational efficiency but also for more strategic applications, such as long-term sustainability goals and predictive market shifts. This trajectory shows the growing importance of AI-driven solutions in maintaining a competitive edge in the evolving industrial landscape.

5. Power-to-X and Machine Learning: A Promising Team-Up

As explored, ML has been successfully used to accelerate the discovery and optimisation of materials, particularly catalysts, essential for scaling PtX technologies and reducing dependency on scarce raw materials. It also enhances predictive modelling to manage fluctuating renewable energy inputs, ensuring seamless system integration and energy management. Economically, ML supports strategic planning and analysis by simulating cost-effective scenarios and improving market viability. Finally, ML plays a crucial role in conducting comprehensive environmental impact assessments, optimising processes to minimise environmental impacts, and ensuring the sustainable development of PtX systems. Together, these capabilities position ML as a cornerstone in advancing PtX technologies towards a more efficient, reliable, and sustainable future.

The structure of this section, which forms the main body of the review, is designed to provide a focused analysis of how machine learning and data-driven methods enhance various Power-to-X processes, with each subsection dedicated to a different PtX technology—Power-to-Gas, Power-to-Liquid, Sustainable Combustion, and Power-to-Heat. This structure allows for a clear, thematic exploration of ML's role in optimising each technology, starting with more established processes like PtG and progressing to more niche applications like PtH.

5.1. Machine Learning & Power-to-Gas Systems

The increasing integration of renewable energy sources into power systems has driven the development of Power-to-X (PtX) technologies, particularly Power-to-Gas (PtG), which convert surplus renewable power into storable forms like hydrogen or methane. Figure 8 represents a schematic of PtG system.

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PtG systems are a technology designed to store surplus renewable energy by converting it into hydrogen or synthetic natural gas (SNG) through electrolysis and methanation processes. In these systems, excess electricity, particularly from intermittent renewable sources like wind or solar, is used to produce hydrogen via water electrolysis. The hydrogen can be stored directly, injected into the natural gas grid, or further converted into SNG by combining it with captured CO_2. PtG systems offer long-term energy storage solutions and can provide flexibility to power grids, reduce wind and solar curtailment, and enhance the integration of renewable energy. Additionally, PtG systems can support ancillary services to the electricity grid, such as frequency and voltage regulation, and facilitate the decarbonisation of sectors such as transportation, heating, and industry [44,45]. They also allow the existing natural gas infrastructure to be used for hydrogen transport and storage, reducing capital investment needs. While PtG systems are still emerging, they show great potential in the transition to a sustainable, low-carbon energy, while ensuring that excess renewable energy is never wasted but instead utilized for further decarbonisation of hard-to-abate sectors.

As the complexity of energy systems grows, machine learning and data-driven methods are becoming central to optimising the efficiency, flexibility, and resilience of PtX systems. This section synthesises insights from several research papers that examine the role of ML in advancing PtG technologies, focusing on the applications of these methods to enhance operational decision-making, uncertainty management, and multi-energy integration.

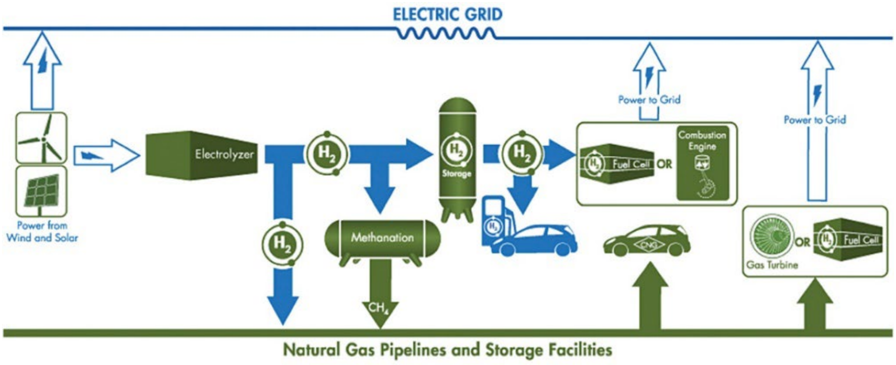

Figure 8. Simplified schematic of a PtG system reprinted with permission from [46].

5.1.1. Coordinating PtG in Multi-Energy Systems

A major theme in PtX research is the use of machine learning to coordinate the interaction between multiple energy carriers—electricity, heat, gas, and hydrogen—particularly in systems that integrate PtG. Y. Zhang et al. (2022) [47] emphasises the need for data-driven robust optimisation to manage the interplay between wind and solar energy outputs in electric-gas networks. Their model employs data-driven robust optimisation (DDRO) techniques to process historical data on renewable generation and create a Minimum Volume Enclosing Ellipsoid (MVEE) uncertainty set, allowing the system to optimise dispatch decisions with reduced conservatism. Similarly, Z. Yang and Jiang (2024) [48] proposed a two-step scheme for multi-energy systems (MES) integrating PtG to mitigate renewable energy curtailment by converting excess wind and solar energy into natural gas. Machine learning, specifically deep neural networks, is trained using historical data to optimise real-time decision-making in electricity-heat demand response (DR), significantly reducing charging costs and improving system security amidst uncertainties in renewable energy supply.

Integration of Combined Cooling, Heating, and Power (CCHP) systems with PtG in multi-energy system has been a key strategy in enhancing the flexibility and reliability of multi-energy systems, according to the literature. This combination leverages renewable energy to meet diverse energy needs—electricity, heating, cooling, and gas—while addressing the uncertainties inherent in wind and solar power. Yang et al. (2023) [49] proposed a two-stage framework that combines CCHP, PtG, and carbon capture, optimising system operations through ML models that generate predictive scenarios based on historical energy imbalances. This approach improves multi-energy coordination at the regional scale, balancing cost and reliability. Siqin et al. (2022) [50] focus on a PtG-CCHP

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microgrid, where uncertainties in wind and solar generation are tackled using a Wasserstein metric in their DRO model. By integrating PtG with CCHP, they enhance system flexibility and reliability, much like Yang's regional framework but applied at a smaller scale. In a similar vein, L. Wang et al. (2024) [51] introduced a novel Power-to-Gas-to-Power (PtG-PtP) system driven by the Allam cycle, which integrates carbon capture and water desalination into PtG processes. By combining exergy analysis with machine learning techniques like Artificial Neural Networks (ANN) and multi-objective optimisation, their system maximises energy and water production efficiencies while reducing emissions, highlighting a novel approach for multi-energy system design in PtG technologies. Also, L. Li et al. (2022) [52] propose a 100% renewable island energy system integrating PtG, biogas, Combined Cooling, Heating, and Power (CCHP), and desalination technologies to meet electricity, heating, cooling, gas, and fresh water demand under extreme weather conditions. The model utilises agent-based modelling (ABM) for energy demand prediction and employs multi-objective optimisation to design and optimise system dispatch using k-means clustering. Results show that compared to battery storage, PtG reduces annual costs by 2.5%, while extreme weather resilience is improved through enhanced biogas and desalination capacities, demonstrating the system's economic and environmental benefits.

Mansouri et al. (2023) [53] integrated real-time IoT data with a deep learning framework using a Long Short-Term Memory (LSTM) neural network to predict energy demand and dynamically adjust energy supply, including PtG in multi-energy microgrids. This enables systems to quickly adapt to fluctuations in market prices and renewable energy availability. Also, Olanlari et al. (2022) [54] used machine learning to optimise multi-energy virtual power plants (MEVPP), coordinating PtG, energy storage, and renewables through an Epsilon-constraint method and a fuzzy satisfying approach. This maximized profits while meeting emissions targets, with machine learning predicting market prices and demand fluctuations to adjust strategies. Meanwhile, Qi et al. (2022) [55] enhanced system reliability by integrating a Power-to-Methane (PtM) system with Liquid CO2 Energy Storage (LCES), balancing renewable energy supply and demand. Zhong et al. (2024) [56] further improved operational flexibility by introducing a PtM system combining solid oxide electrolysis cells (SOEC) and a methanation reactor, optimising off-design performance to enhance efficiency.

5.1.2. Deep Reinforcement Learning for Dynamic Optimisation

The dynamic nature of renewable energy generation requires real-time decision-making, and deep reinforcement learning (DRL) has proven to be particularly effective in handling such challenges. Liang et al. (2024) [57] and B. Zhang et al. (2023) [58] both apply DRL algorithms to PtG systems, integrating them with carbon capture technologies.

Liang et al. (2024) [57] implemented a Twin Delayed Deep Deterministic Policy Gradient (TD3) algorithm to dynamically optimise energy flows in complex systems, providing stability and adaptability through continuous action spaces. B. Zhang et al. (2023) [58] enhanced this approach by using a Soft Actor-Critic (SAC) algorithm with prioritized experience replay, improving learning efficiency and enabling quicker adaptation to fluctuations in renewable generation and market prices. Similarly, Cui et al. (2023) [59] applied the SAC algorithm to optimise electricity-gas-heat coupling in low-carbon microgrids, incorporating Power-to-Gas (PtG) and Organic Rankine Cycle (ORC) technologies. Wen and Aziz (2023) [60] further explored energy hub scheduling using a modified double deep Q-network, comparing power-to-gas-to-power (PtX2P) and biomass-to-gas-to-power (B2X2P), with B2X2P proving more profitable but PtX2P offering greater flexibility. Finally, Monfaredi et al. (2023) [61] introduced a multi-agent deep reinforcement learning (MA-DRL) method to optimise energy management in microgrids, improving coordination of renewable energy resources and reducing both operational costs and carbon emissions.

These studies collectively demonstrate the effectiveness of advanced reinforcement learning algorithms, such as TD3, SAC, and multi-agent DRL, in optimising energy flows and improving the operational flexibility of multi-energy systems. By incorporating real-time adaptability and advanced coordination of energy resources, these methods not only enhance system efficiency but also reduce

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operational costs and carbon emissions, making them vital for managing the complexities of renewable energy integration in PtG systems and multi-energy microgrids.

5.1.3. Predictive Diagnostics in PtG Systems

In addition to optimisation, machine learning enhances the reliability of PtG systems through predictive diagnostics. Zaveri et al. (2023) [62] developed a machine learning-based diagnostic model for proton exchange membrane fuel cells (PEMFCs), used in PtG systems to produce hydrogen. By employing supervised learning algorithms, including advanced regression techniques, such as support vector machine, decision tree regression, random forest regression and artificial neural network, they detect early signs of PEMFC malfunction, such as dehydration or flooding. The predictive capabilities of these models improve system reliability and reduce downtime, ensuring the consistent production of hydrogen in PtG applications. Ma et al. (2022) [63] also focus on PEMFC systems integrated with PtG, but in the context of hybrid energy systems that address renewable uncertainty. Their study applies wavelet transform-neural network to optimise PEMFC operations under fluctuating renewable inputs, ensuring that energy storage and hydrogen production remain stable. The integration of PEMFC and PtG, supported by machine learning, enables these systems to balance renewable energy variability effectively.

ML improves the reliability of PtG systems, particularly through predictive diagnostics for PEMFCs, as demonstrated by Zaveri et al. (2023) [62], who used various supervised learning algorithms to detect early signs of malfunction. Additionally, the wavelet transform-neural network approach by Ma et al. (2022) [63] ensures stable PEMFC operations in hybrid systems by balancing renewable energy fluctuations. These advancements ensure consistent hydrogen production and enhance the operational stability of PtG systems.

5.1.4. Market Integration and Carbon Capture in PtG Systems

Machine learning has also been applied to optimise PtG systems in the context of market operations, particularly in integrating carbon trading mechanisms and electricity markets. Researchers has attempted to make PtG systems economically viable in competitive market environments by applying machine learning; X. Zheng et al. (2021) [64] proposed a stochastic co-optimisation model for power-gas systems in day-ahead markets. Their model integrates PtG technologies and uses machine learning-based methods, such as Gaussian Process Regression (GPR), to predict electricity and gas prices. Also, Janke et al. (2020) [65] explored bidding strategies for Power-to-X (PtX) systems in day-ahead electricity markets, utilising an artificial neural network (ANN) to forecast electricity prices and develop a price-independent order (PIO) strategy. While PIO helps avoid expensive, carbon-intensive electricity during peak loads, it results in fewer operating hours and higher hydrogen production costs compared to a price-dependent order (PDO), which proved to have 10.9% lower levelised hydrogen costs.

Li et al. (2023) [66] extended the application of machine learning to near-zero carbon emission power plants (NZCEP), integrating PtG and CCS to optimise both energy production and carbon capture under carbon trading mechanisms. Their use of a K-means clustering algorithm simplified carbon pricing scenarios and optimised operations based on real-time carbon price signals. Similarly, Wu and Li (2023) [67] incorporated PtG into hydrogen-based integrated energy systems with CCS, utilizing a Wasserstein-based DRO model and machine learning predictions to manage fluctuations in renewable generation and carbon prices. This approach efficiently converts surplus renewable energy into hydrogen while capturing and storing carbon emissions. Lastly, Janke et al. (2020) [65] focused on optimising Power-to-Hydrogen systems by developing a price-independent order (PIO) bidding strategy for the electricity market. Supported by artificial neural networks (ANN), this strategy improved electricity price forecasting and reduced hydrogen production costs by avoiding peak demand periods. Despite the price-dependent order (PDO) strategy offering lower levelized costs overall, PIO proved effective under volatile market conditions, providing a valuable tool for plant operations. Together, these advancements highlight how machine learning and advanced strategies can enhance the efficiency and adaptability of PtG systems in various operational contexts.

5.1.5. Handling Uncertainty with Data-Driven Robust Optimisation

Uncertainty management is a recurring theme across many of these studies, regardless of the specific focus. Whether managing renewable energy variability or dealing with market price fluctuations, machine learning is central to building models that can anticipate and respond to unpredictability. The use of distributionally robust optimisation (DRO) by Siqin et al. (2022) [50], Yang et al. (2023) Yang et al. (2023), and L. Zheng et al. (2024) [68] showcases how robust models can mitigate risks associated with wind and solar generation. Similarly, deep reinforcement learning (DRL), as used by Liang et al. (2024) [57] and B. Zhang et al. (2023) [58], allows for real-time adaptation to fluctuating energy supply and demand. In predictive diagnostics, Zaveri et al. (2023) [62] and Ma et al. (2022) [63] demonstrate how machine learning can anticipate failures in PEMFCs, improving system stability.

Also, Fan et al. (2023) [69] developed a two-stage distributionally robust optimisation (TSDRO) model for integrated energy system groups (IESG), focusing on energy sharing and carbon transfer under wind and photovoltaic power uncertainties. The model utilises kernel density estimation (KDE) and the Wasserstein metric to construct fuzzy uncertainty sets, achieving a balance between robustness and economic efficiency. Similarly, Gao et al. (2022) [70] introduced a data-driven DDRO model for urban integrated energy systems, focusing on wind power uncertainty. They employed techniques such as KDE and the Wasserstein metric to improve resource utilisation and system robustness in PtG applications.

The application of machine learning in PtG systems has addressed key challenges such as optimising energy flows, managing uncertainty, and integrating multi-energy systems. Studies utilising techniques like deep reinforcement learning, distributionally robust optimisation, and predictive diagnostics have demonstrated improvements in system flexibility, reliability, and operational efficiency. The studies, however, could not be limited to the proposed categorisation as the applications of ML could be so diverse and innovative, still related to the field. For example, Lakhmi et al. (2024) [71] presented another use of ML in process monitoring, focusing on a gas sensor array designed to control PtX processes. Using both linear models (Partial Least Squares) and non-linear models (ANN), they showed that ANN models provided more accurate predictions for methane concentrations, offering superior performance for process control applications.

Furthermore, machine learning has shown potential in enhancing market integration and handling renewable energy variability. The literature, as summarized in the Table 1, suggests that as PtG systems grow more complex, machine learning will be crucial in advancing their capabilities to meet future energy demands and decarbonisation goals.

Table 1. Key Findings from Recent Literature on Machine Learning & Power-to-Gas Systems.

Paper	Focus Area	ML Method Used	Application	Key Contribution
Zhang et al. (2022) [47]	Integrated electric-gas systems	Data-driven robust optimisation (DDRO), Minimum Volume Enclosing Ellipsoid (MVEE)	Wind-solar output correlation in IEGS	Proposes a two-stage dispatch model for integrated electric-gas systems, improving day-ahead and real-time dispatch costs with MVEE uncertainty set.
Yang and Jiang (2023) [48]	Multi-Energy Systems (MES)	Deep Neural Networks (DNN)	Real-time decision-making for integrated heat-electricity demand response (DR)	Reduced charging costs and optimised real-time operational decisions without prior knowledge of future conditions. Integrated PtG to

				reduce renewable energy curtailment.
Yang et al. (2023) [49]	Regional integrated energy systems (RIES)	Data-driven two-stage DRO	CCHP-PtG-CCS planning under uncertainty	Uses DRO for planning regional CCHP-PtG-CCS systems, improving reliability and reducing carbon emissions under multi-energy uncertainty.
Siqin et al. (2022) [50]	PtG-CCHP microgrid	Distributionally robust optimisation (DRO), Wasserstein metric	Economic dispatch under uncertainty	Proposes a PtG-CCHP system with DRO to improve stability, economy, and low-carbon operation by managing wind and solar uncertainty.
Wang et al. (2024) [51]	Power-to-Gas-to-Power (PtG-PtP) and Carbon Capture	Artificial Neural Networks (ANN), Multi-Objective Optimization	Integration of PtG-PtP with the Allam cycle for simultaneous electricity and water production	Proposed a novel system combining PtG with the Allam cycle for energy generation, carbon capture, and water desalination, optimizing exergy efficiency and minimizing emissions
Li et al. (2022) [52]	Island energy systems	Agent-based modelling (ABM), k-means clustering	100% renewable island with PtG	Proposes a multi-objective optimisation for island energy systems integrating PtG and desalination technologies, reducing costs and improving weather resilience.
Mansouri et al. (2023) [53]	Multi-energy microgrids	Long Short-Term Memory (LSTM), IoT-based prediction	Market management for smart prosumers	Proposes an IoT-enabled hierarchical framework for multi-energy microgrid market management using deep learning to optimise demand response strategies.
Ghasemi Olanlari et al. (2022) [54]	Multi-energy virtual power plants (MEVPP)	Fuzzy satisfying approach, Epsilon-constraint method	VPP with PtG and demand response integration	Develops an optimal scheduling model for MEVPP integrating PtG, renewable energy, and demand response to maximise

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				profit and minimise emissions.
Qi et al. (2022) [55]	Energy storage in PtM process, techno-economic evaluation	Artificial neural network-based surrogate optimization	Design and optimization of the PtM-LCES process using a renewable power mix	Demonstrated that integrating LCES in the PtM process enhances profitability and energy efficiency, and reduces methane production costs, making it competitive with fossil natural gas.
Zhong et al. (2024) [56]	Power-to-Methane (PtM) with SOEC integration	No specific ML method, focuses on optimisation algorithms	Solid oxide electrolysis and methanation reactor optimisation	Optimised off-design performance of Power-to-Methane systems, enhancing operational flexibility and efficiency.
Liang et al. (2024) [57]	Integrated energy system with CCS-PtG	Twin Delayed Deep Deterministic Policy Gradient (TD3)	Real-time scheduling for low-carbon energy	Uses DRL to dynamically optimise scheduling in CCS-PtG systems, lowering carbon emissions and operational costs.
B. Zhang et al. (2023) [58]	Integrated CCS and PtG systems	Soft Actor-Critic (SAC) with Prioritized Experience Replay (PER)	Dynamic energy dispatch optimisation	Improved system flexibility and reduced operational costs through SAC-based real-time optimisation in CCS-PtG systems.
Cui et al. (2023)	Low-carbon economic dispatch of microgrid	Soft Actor-Critic (SAC), Multilayer Perceptron (MLP)	Electricity-gas-heat coupling with PtG	Proposes a low-carbon dispatch model with SAC to reduce microgrid CO2 emissions and operational costs by optimising electricity-gas-heat coupling and PtG.
Wen and Aziz (2023) [59]	CCS and PtG integration	Multi-agent reinforcement learning (MARL)	Carbon capture and energy system optimisation	Proposes a model for integrating carbon capture and PtG systems using MARL to optimise energy management and reduce emissions in energy systems.
Monfaredi et al. (2023) [61]	Optimal Energy Management in Microgrids	Multi-Agent Deep Reinforcement Learning (MA-DRL)	Energy management in grid-connected microgrids	Developed a robust MA-DRL-based strategy to coordinate multiple energy

				carriers, reducing emissions and costs while optimising microgrid operations.
Zaveri et al. (2023) [62]	PEM Fuel Cells (PEMFC) in PtG systems	Support Vector Machine (SVM), Decision Tree, Random Forest, ANN	PEMFC diagnostics for failure prediction	Machine learning model predicts PEMFC failures like dehydration and flooding, improving reliability and stability in PtG systems.
Ma et al. (2022) [63]	Hybrid PEMFC-PtG systems	Wavelet transform-neural network	PEMFC-PtG under renewable uncertainty	Proposes a hybrid PEMFC-PtG system optimised with ML for renewable integration, reducing operating costs and emissions.
Zheng et al. (2021) [64]	Electricity-gas systems	Stochastic co-optimisation, Sequential Mixed-Integer Second-Order Cone Programming (SOC)	Day-ahead market participation	Co-optimises electricity and gas systems in day-ahead markets under uncertainty using PtG, with new pricing and settlement mechanisms.
Janke et al. (2020) [65]	Power-to-X (PtX) systems	Artificial Neural Network (ANN)	Electricity price forecasting	Developed price-independent order (PIO) strategy for hydrogen production to optimise bidding strategies in day-ahead markets
Zheng et al. (2024) [68]	Multi-energy systems under uncertainty	Clayton copula-based joint probability distribution, DRO	Uncertainty management in carbon-electricity markets	Proposes a DRO model for coordinating MES interactions and mitigating uncertainty in carbon and electricity markets using PtG integration.
Li et al. (2023) [66]	Near-zero carbon emission power plants (NZCEP)	K-means clustering, Data-driven robust optimisation (DSRO)	Scheduling under electricity-carbon markets	Proposes a DSRO model for scheduling NZCEPs, optimising renewable energy consumption and carbon credit generation under electricity-carbon market.

Wu and Li (2023) [67]	Hydrogen-based integrated energy systems (HIES)	Wasserstein metric-based DRO	HIES with PtG and carbon trading	Proposes a WDRO model for optimising HIES with PtG and CCS under carbon trading and renewable uncertainty, reducing operational costs and emissions.
Fan et al. (2023) [69]	Integrated energy systems (IES)	Kernel Density Estimation (KDE), Wasserstein metric	Energy sharing and carbon transfer optimisation	Develops a two-stage DRO for energy sharing and carbon transfer in IES, reducing carbon emissions and improving resource allocation with CCUS and PtG integration.
Gao et al. (2022) [70]	Urban integrated energy systems (UIES)	Distributionally robust optimisation (DRO), Norm-1 and Norm-inf constraints	UIES with wind power uncertainty	Proposes a DDRO model for urban integrated energy systems, optimising energy purchases and mitigating wind power uncertainty using norm-based constraints.
Lakhmi et al. (2024) [71]	Process Control in Power-to-X Systems	Artificial Neural Network (ANN), Partial Least Squares (PLS)	Gas sensor array for process control and gas mixture composition detection	Built sensor arrays for monitoring gases in Power-to-X systems; ANN proved more effective for methane detection than linear models.

5.2. Machine Learning & Power-to-Liquid Systems

Power-to-Liquid (PtL) systems are an innovative approach to converting renewable energy into liquid fuels, utilising surplus electricity to synthesize hydrocarbons, methanol, and ammonia. These processes typically involve using renewable electricity for water electrolysis to produce hydrogen, which is then combined with captured CO_2 in processes like Fischer-Tropsch synthesis to create carbon-neutral fuels such as methanol or synthetic diesel. Ammonia is also increasingly produced in PtL systems, serving as a carbon-free hydrogen carrier with advantages in storage and transportation. Recent advancements, such as plasma-assisted ammonia synthesis, enhance the efficiency of ammonia production at lower temperatures and pressures, reducing the energy footprint [72,73]. PtL fuels can be seamlessly integrated into existing fuel infrastructure, supporting decarbonisation in sectors like aviation, shipping, and heavy industry. These systems offer flexibility in fuel production while helping close the carbon cycle by using captured CO_2 or nitrogen, making them a key solution for achieving net-zero emissions in hard-to-abate sectors.

Green ammonia is emerging as a key hydrogen carrier due to its high hydrogen content, low flammability, and established transport infrastructure, making it vital for industries such as fertilizers and fuel cells. Its potential to reduce energy consumption and emissions is significant. Catalytic decomposition using nickel-based catalysts is noted for its cost-effectiveness in large-scale hydrogen production, and machine learning aids in optimising these catalysts by simulating reaction mechanisms [74,75]. Recent advancements in green ammonia synthesis emphasize its role in sustainable energy due to its low-carbon footprint and compatibility with renewable energy sources. Deng et al. (2024) [75] proposed a physics-informed sparse identification model for optimising reactor design, enhancing ammonia yield using a bald eagle search algorithm. Similarly, Zeng et al. (2023) [76] employed plasma catalysis under low-temperature pulsed plasmas, optimising parameters through a Bayesian neural network to improve energy efficiency. These studies collectively advance green ammonia synthesis by integrating machine learning and optimisation techniques to boost yield and sustainability. A schematic of green ammonia synthesis process is shown in Figure 10.

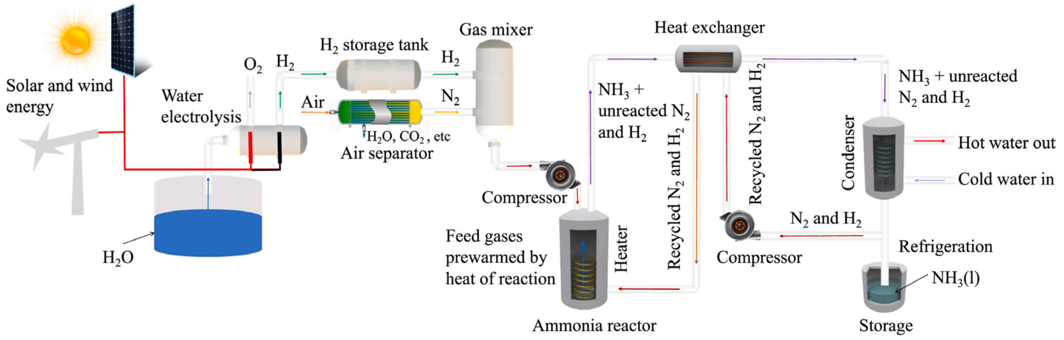

Figure 10. schematic of green ammonia synthesis process. Reprinted with permission from [75].

Power-to-Ammonia (PtA) technology provides a practical solution for converting surplus renewable energy into ammonia, a fuel that is both storable and transportable, offering a means to enhance the stability of multi-energy systems. In recent research, PtA is being integrated into energy hubs that combine renewable power sources with advanced energy storage and management systems. These hubs are optimised to address the intermittent nature of renewable energy by converting it into green ammonia, which can later be used for power generation or other applications. In this context, studies have focused on designing energy-efficient, cost-effective solutions to improve the operation of PtA systems within multi-energy hubs, particularly in terms of energy conversion efficiency and system scalability [77,78]. Innovations in PtA system integration are not only improving energy efficiency but also unlocking new strategies for managing complex energy flows in real-time. By leveraging advanced optimisation algorithms, such as deep reinforcement learning, these systems are becoming increasingly adept at responding to the variability of renewable energy, as demonstrated by recent studies.

In their study, Xiong et al. (2023) [77] propose a coordinated energy management strategy for a renewable-powered multi-energy hub that incorporates PtA technology. Their system employs a multi-agent deep reinforcement learning (DRL) algorithm to optimise energy flow, ensuring that the hub can efficiently handle fluctuating renewable energy inputs, such as wind and solar. The use of the DRL algorithm significantly enhances the hub's ability to minimise operational costs and carbon dioxide emissions, while also maximising ammonia production. On the other hand Qi et al. (2022) [78] presented a different approach by proposing an energy hub that integrates PtA with liquid air energy storage (LAES) technology. Their system is designed to co-produce green ammonia and electricity, using a surrogate-based optimisation method to achieve cost-optimal configurations. By combining LAES with PtA, the system enhances its flexibility and performance, allowing it to store excess renewable energy and generate power on demand.

Ammonia-fueled solid oxide fuel cells (SOFCs) offer the ability to directly convert ammonia into electricity with high efficiency and lower carbon emissions. These systems are particularly attractive due to ammonia's high energy density and ease of storage compared to hydrogen. However, challenges remain in optimising their performance, particularly in managing the high temperatures generated during ammonia decomposition and improving overall system efficiency. Yanchen Lai et al. (2023) [79] have addressed this by investigating the thermal management of ammonia-fueled tubular SOFCs, focusing on the impact of ammonia cracking reactions within the fuel cell. Their study develops a thermal management model, proposing pre-reforming techniques and optimised reaction activation energy to improve temperature distribution and reduce thermal stress. Meanwhile, Y. Du et al. (2023) [80] propose a novel SOFC and rotary engine system, integrating hydrogen regeneration to enhance part-load performance. Using a data-driven model, they optimise the system's efficiency, showing significant improvements in energy output, particularly at partial loads.

While ammonia has gained significant attention in PtL technologies, PtL systems are versatile and can produce a variety of fuels, including hydrogen, methanol, and hydrocarbons. Recent research has focused on optimising these systems using machine learning and advanced optimisation techniques to enhance their efficiency and flexibility. For example, Ahbabi Saray et al. (2024) [81] developed a system that produces both liquid hydrogen and ammonia using renewable energy, employing artificial neural networks (ANNs) and genetic algorithms (GA) for optimisation. Their system not only efficiently balances the production of hydrogen and ammonia but also addresses multiple energy needs, such as cooling and freshwater generation. Also, Zhao et al. (2024) [82] focus on hydrogen production through solar-assisted methanol steam reforming, optimising key operational factors using a GA-Back Propagation Neural Network (GA-BPNN) model. Expanding PtL beyond ammonia and hydrogen, Mohammad Nezhad et al. (2024) [83] optimised a Fischer-Tropsch process for hydrocarbon fuel production in small-scale PtL plants. Using surrogate models and genetic algorithms, they enhance the efficiency of the fuel production system, which offers a compact and localised energy storage solution. The key findings related to ML applications in Power-to-Liquid Systems are summarised in **Table 2**.

Table 2. Key Findings from Recent Literature on Machine Learning & Power-to-Liquid Systems.

Paper	Focus Area	ML Method Used	Application	Key Contribution
Deng et al. (2024) [75]	Green ammonia synthesis	Bald eagle search algorithm, sparse identification	Optimising ammonia reactor design	Improved ammonia yield by optimising reactor parameters using time-series data analysis.
Zeng et al. (2023) [76]	Plasma-assisted ammonia synthesis	Bayesian Neural Network (BNN)	Optimising plasma catalysis for ammonia production	Enhanced energy efficiency through pulse voltage and gap optimisation.
Xiong et al. (2023) [77]	Power-to-Ammonia in multi-energy hubs	Deep Reinforcement Learning (DRL)	Energy flow optimisation in multi-energy hubs	Maximised ammonia production and minimised operational costs with renewable energy.
Qi et al. (2022) [78]	Power-to-Ammonia with LAES integration	Surrogate-based optimisation	Co-production of green ammonia and electricity	Achieved cost-optimal system configuration and enhanced flexibility.
Lai et al. (2023) [79]	Ammonia-fueled solid oxide fuel cells	No ML used; thermal management model analysis	Optimising SOFC performance for ammonia fuel	Developed a thermal management model to improve temperature

				distribution in SOFCs.
Du et al. (2023) [80]	SOFC and rotary engine systems	Data-driven model using optimisation algorithms	Part-load performance optimisation for SOFC systems	Improved energy output and efficiency, especially under partial loads.
Ahbabi Saray et al. (2024) [81]	Dual hydrogen and ammonia production	Artificial Neural Network (ANN), Genetic Algorithm (GA)	Renewable-powered hydrogen and ammonia co-production	Balanced hydrogen and ammonia production with optimised energy system performance.
Zhao et al. (2024) [82]	Hydrogen production from methanol	GA-Back Propagation Neural Network (GA-BPNN)	Solar-assisted methanol steam reforming for hydrogen production	Optimised operational parameters for enhanced hydrogen yield and system efficiency.
Mohammad Nezhad et al. (2024) [83]	Fischer-Tropsch fuel production	Surrogate model, Genetic Algorithm (GA)	Small-scale hydrocarbon fuel production	Optimised Fischer-Tropsch process, enhancing the efficiency of localised fuel storage.
Mashhadimoslem et al. (2023) [74]	Green ammonia synthesis using nickel-based catalysts	Machine learning for catalyst optimisation	Catalytic decomposition in green ammonia production	Used ML to optimise nickel-based catalysts for hydrogen production, improving efficiency and reducing costs.

5.3. Advances in Sustainable Combustion and Fuel Optimisation for Next-Generation Engines

The transition to sustainable combustion will depend heavily on the interplay between hydrogen and carbon-based fuels, each offering unique advantages and challenges. Hydrogen's potential as a clean fuel is promising due to its versatility and low carbon footprint, but its combustion presents technical hurdles, such as flame instability and nitrogen oxide emissions. Meanwhile, carbon-based fuels, especially those derived from renewable sources, provide higher energy densities, making them indispensable for sectors like aviation. However, their reliance on carbon capture and the complexity of their combustion processes necessitate advanced computational methods, including ML, for optimising fuel efficiency and minimising emissions. As highlighted by Pitsch (2024) [84], both hydrogen and carbon-based fuels require innovative approaches in fuel technology and computational modelling to drive the transition towards sustainable combustion.

To fully leverage hydrogen's potential as a clean fuel, its production and distribution systems must be optimised. In particular, managing hydrogen refueling stations is critical, where fluctuating demand and integration with renewable energy sources create operational challenges. Huy et al. (2024) [85] address this issue by implementing Generative Adversarial Imitation Learning (GAIL) to

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optimise real-time energy management, improving decision-making by mimicking expert strategies to balance hydrogen production with electricity generation.

ML's role in combustion modelling is equally crucial, particularly for hydrogen- and carbon-based fuels. Traditional computational models struggle with non-linear interactions like flame instability, but ML offers a solution by enhancing combustion simulations with data-driven approaches. As Pitsch (2024) [84] notes, integrating ML with physics-based models is essential for optimising fuel design, enhancing combustion efficiency, and reducing emissions. Expanding on this, Kale et al. (2023) [86] explored the stability of hydrogen-CNG powered vehicles, using advanced control techniques such as MIMO system models and transfer functions to ensure operational feasibility in hybrid fuel systems.

Recent advancements in engine design further underscore the importance of ML in combustion systems. Sapra et al. (2024) [87] applied computational fluid dynamics (CFD) and Gaussian Process Regression (GPR) to optimise piston-bowl geometries for energy-assisted compression ignition using low-cetane sustainable aviation fuel blends. This integration significantly reduces ignition delays and improves fuel efficiency, particularly under high-altitude and high-load conditions. Similarly, Narayanan et al. (2024) [88] developed the Misfire-Integrated Gaussian Process (MInt-GP) emulator to enhance control systems for jet fuels with varying cetane numbers, offering up to 80 times faster computation than traditional CFD methods, which reduces the cost and time associated with engine control system training.

Finally, ML plays a key role in evaluating the environmental impact of alternative fuels. Ahmed et al. (2023) [89] used supervised ML models, including Random Forest, Decision Tree, and XGBoost, to assess the life cycle impact of offshore vessels powered by LNG and green ammonia. The study found that green ammonia-powered vessels exhibited lower global warming potential and emissions compared to conventional fuels, with XGBoost outperforming other models in predictive accuracy, providing a robust framework for environmental impact assessments.

5.3.1. Sustainable Aviation Fuel (SAF)

Production of sustainable liquid fuels can be classified under PtL processes. According to L. Yang et al. (2023) [90], who presented a comprehensive framework to quantify CO_2 emissions from China's civil aviation industry up to 2050 by using a combination of Backpropagation Neural Network (BPNN) and Monte Carlo simulations, addressing the uncertainties in future aviation demand and policy changes is crucial for meeting decarbonisation goals. Their analysis shows that while sustainable aviation fuels (SAFs) are pivotal to reducing emissions, achieving carbon neutrality by 2050 will require SAFs to account for up to 70% of aviation fuel. In addition to SAF adoption, innovations in aircraft technology, carbon capture methods, and carbon trading mechanisms will be essential to offset emissions and meet global targets. This highlights the growing role of machine learning in not only forecasting emissions but also optimising the integration of SAFs into the aviation fuel mix.

In line with these findings, F. Wang and Rijal (2024) [91] further explored the potential of sustainable aviation fuels by focusing on strained hydrocarbons and cycloalkanes as promising SAF candidates due to their high energy density and efficient combustion properties. Their study employs machine learning techniques such as quantum chemistry-based simulations and neural networks to optimise molecular structures, enhancing fuel stability, energy density, and combustion efficiency. They emphasized the importance of addressing production challenges, providing a detailed technoeconomic assessment based on life cycle assessment (LCA) and production cost models, which evaluate the scalability and economic viability of SAF production. While their results show that these SAFs offer significant performance advantages, scaling up production remains a challenge due to high initial costs.

The key findings related to on the applications of ML in Sustainable Aviation fuels are summarised in Table 3.

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Table 3. Key Findings from Recent Literature on the applications of ML in Sustainable Aviation fuel (SAF).

Paper	Focus Area	ML Method Used	Application	Key Contribution
Pitsch (2024) [84]	Hydrogen and Carbon-based Fuel Combustion	Data-driven modelling	Combustion simulations for hydrogen and carbon-based fuels	Integrated ML and physics-based models to address non-linear interactions in turbulent combustion, enhancing fuel efficiency and reducing emissions.
Huy et al. (2024) [85]	Hydrogen Refueling Station Optimisation	Generative Adversarial Imitation Learning (GAIL)	Real-time energy management in hydrogen refueling stations	Developed an ML-based energy management model that mimics expert strategies to optimise hydrogen production and electricity generation, improving efficiency and flexibility.
Kale et al. (2023) [86]	Hydrogen-CNG Hybrid Vehicles	MIMO system models, Bode plots	Stability analysis of hydrogen-CNG powered vehicles	Analyzed vehicle stability and control using transfer functions to ensure the operational feasibility of hydrogen-CNG hybrid fuel systems.
Sapra et al. (2024) [87]	Engine Design for Low-Cetane Aviation Fuels	Gaussian Process Regression (GPR)	Piston-bowl design optimisation for low-cetane fuel blends	Combined CFD and ML to optimise engine geometries, reducing ignition delays and enhancing fuel efficiency in sustainable aviation fuel blends.
Narayanan et al. (2024) [88]	Energy-Assisted Compression Ignition (EACI) Engines	Misfire-Integrated Gaussian Process (MInt-GP)	Control system optimisation for varying cetane number jet fuels	Developed a physics-integrated GP model to predict combustion profiles, offering up to 80 times faster computation than CFD, improving control system training.
Yang et al. (2023) [90]	Sustainable Aviation Fuel (SAF) Emissions	Backpropagation Neural Network (BPNN), Monte Carlo	CO_2 emission quantification in China's civil aviation industry	Used ML to address uncertainties in aviation demand and policy, showing SAFs must account for up to 70% of aviation fuel to

				meet decarbonisation goals.
Wang and Rijal (2024) [91]	SAF Development and Optimisation	Neural Networks, Quantum Chemistry-Based Simulations	Optimisation of SAF molecular structures (strained hydrocarbons and cycloalkanes)	Employed ML to optimise fuel molecular structures, enhancing SAF stability and combustion efficiency, while providing a techno-economic assessment of SAF scalability.

5.4. Machine Learning and Power-to-Heat

Power-to-Heat (PtH) systems convert excess electricity, typically from renewable sources like wind or solar, into heat, which can be used for space heating, industrial processes, or stored in district heating systems. These systems help balance electricity grids by utilising surplus energy during periods of high renewable generation and low demand. PtH technologies, such as electric boilers and heat pumps, can be integrated into district heating networks, providing flexibility by shifting energy between the electricity and heat sectors. Furthermore, as highlighted in recent studies Liu et al. (2023) [92], buildings themselves can offer flexibility services to the grid by integrating PtH systems with model predictive control and leveraging thermal inertia. This allows buildings to modulate energy consumption in response to fluctuating energy prices and renewable availability, further enhancing grid stability. By replacing fossil-fuel-based heat production, PtH technologies contribute to decarbonisation and reduce greenhouse gas emissions in the heating sector. Studies have shown that PtH systems can significantly reduce wind and solar curtailment and lower operational costs for energy systems, especially when integrated with thermal storage [93,94].

In their study Liu et al. (2023) [92] emphasized the application of machine learning, particularly model predictive control (MPC), in optimising Power-to-Heat (PtH) systems to provide flexibility services within building energy systems. By using MPC, these systems can adjust energy consumption dynamically based on real-time data, responding efficiently to variations in renewable energy supply and electricity demand. The demand-side flexibility has been a concern in other studies as well; Nunna et al. (2023) [95] also explored demand-side flexibility in ultra-low temperature district heating (ULTDH) systems using Power-to-Heat solutions. By applying a genetic algorithm (GA) for optimising the charging of hot water storage based on electricity price signals and demand forecasts, the system achieves significant cost savings and energy flexibility. The approach enhances renewable energy integration, demonstrating over 91% cost reduction compared to traditional controls while supporting grid stability. Similarly, the study by Fleschutz et al. (2023) [96] investigates the transition of manufacturing companies from energy prosumers to "flexumers" by leveraging demand-side flexibility within multi-energy systems (MESs). By integrating flexible energy storage and demand response (DR) programs, the study demonstrates how MESs can dynamically adjust their energy profiles, achieving significant reductions in both operational costs and carbon emissions.

The integration of machine learning and data-driven techniques in Power-to-Heat (PtH) systems continues to demonstrate significant potential; the study by Kansara et al. (2024) [97] focuses on integrating physics-driven and data-driven modelling approaches to optimise energy systems that include Power-to-Heat integrated with renewable sources like solar and wind, as well as storage components like thermal energy storage (TES). A key takeaway is that combining both modelling methods can significantly reduce computational time—up to 37% for energy concepts without TES—while maintaining high solution accuracy, offering a balanced trade-off between computational efficiency and precision. Also, Lange and Kaltschmitt (2022) [98] presented a machine learning-based method, using long short-term memory (LSTM) networks, to perform probabilistic day-ahead forecasts of thermal storage capacities in residential Power-to-Heat (PtH) systems. By predicting temperature distributions and transforming them into storage capacity forecasts, the approach improves renewable energy integration, outperforming traditional models in accuracy and reliability. The key findings related to on the applications of ML in Power-to-Heat systems are summarised in Table 4.

Table 4. Key Findings from Recent Literature on Machine Learning & Power-to-Heat Systems.

Paper	Focus Area	ML Method Used	Application	Key Contribution
Liu et al. (2023) [92]	Power-to-Heat systems in building energy flexibility	Model Predictive Control (MPC)	Flexibility services for buildings	Use of MPC to dynamically adjust energy consumption in response to real-time data, enhancing energy flexibility in building systems and renewable energy integration.
Nunna et al. (2023) [95]	Ultra-low temperature district heating (ULTDH)	Genetic Algorithm (GA)	Optimising hot water storage charging and electricity price signals	Demonstrated significant cost savings and enhanced demand-side flexibility by integrating Power-to-Heat systems with district heating using GA-based optimisation.
Fleschutz et al. (2023) [96]	Multi-energy systems (MES) flexibility	Not explicitly ML, focus on demand-side flexibility	MES in manufacturing companies, integrating flexible energy storage	Highlights the transition of companies from energy prosumers to flexumers, using demand-side flexibility for cost and emission reductions.
Lange and Kaltschmitt (2022) [98]	Power-to-Heat residential storage systems	Long Short-Term Memory (LSTM)	Day-ahead probabilistic forecasts of storage capacities	Improved the accuracy and reliability of renewable energy integration through LSTM-based forecasts, optimising thermal storage operations in PtH systems.
Kansara et al. (2024) [97]	Energy system optimisation with Power-to-Heat	Hybrid (Physics-driven and Data-driven models)	Power-to-Heat systems integrated with renewable sources	Achieved 37% reduction in computational time for system optimisation without compromising solution accuracy, using a hybrid modelling approach.

6. Discussion and Insight

The integration of Machine Learning into Power-to-X processes marks a significant evolution in renewable energy management, and offers new opportunities for enhancing system efficiency, flexibility, and sustainability. As PtX technologies grow in complexity, particularly with the

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increasing adoption of renewable energy sources, ML provides advanced tools to optimise performance, facilitate integration, reduce emissions, and handle the inherent uncertainties in energy supply and demand. In this section, we explore the critical findings, implications, limitations, and future directions of ML applications in PtX systems for a comprehensive overview of the field's current state and its trajectory toward future innovations.

6.1. Summary of Key Findings

This review identifies several crucial advancements in the integration of ML/Data-driven methods with PtX processes, spanning from Power-to-Gas (PtG) and Power-to-Liquid (PtL) to Power-to-Heat (PtH) systems. One of the main findings is that ML enhances system optimisation, improving overall efficiency in energy conversion, system integrations, and storage processes. In Power-to-Gas systems, ML-based models such as deep reinforcement learning and robust optimisation algorithms have significantly improved real-time operational decision-making, reducing both operational costs and carbon emissions. Studies show that ML's predictive diagnostics and dynamic optimisation capabilities are instrumental in managing uncertainties inherent in renewable energy systems, particularly in fluctuating renewable energy inputs like wind and solar power.

Similarly, in Power-to-Liquid processes, ML models have been applied to optimise ammonia and synthetic fuel production processes. This enables improved efficiency in renewable hydrogen production, which is combined with CO_2 to generate liquid fuels via processes such as Fischer-Tropsch synthesis. Studies highlight how ML aids in optimising the performance of renewable-based energy hubs that integrate Power-to-Ammonia (PtA) systems, improving energy storage and flexibility.

In Power-to-Heat systems, the application of ML, particularly model predictive control (MPC), enhances energy efficiency by dynamically adjusting heating demand based on real-time data and renewable energy supply. This approach has significantly contributed to reducing grid curtailment and improving renewable energy integration into district heating systems.

These findings have far-reaching implications for the energy transition, particularly in integrating renewable energy systems with flexible storage and energy conversion technologies. By improving the efficiency, reliability, and flexibility of PtX systems, ML offers new insights into overcoming the challenges of renewable energy intermittency. For example, ML-enhanced PtX processes help align energy production with demand, addressing the imbalance between energy supply and demand, particularly in multi-energy and integrated systems, across multiple timescales. This has also direct applications in industrial sectors, heavy transportation, and aviation, where energy storage and conversion challenges are more pronounced.

ML-based models also provide robust solutions for managing the complexities of carbon capture and storage (CCS) integration with PtX systems. This integration is vital for decarbonising sectors that rely heavily on fossil fuels. The ability of ML to forecast energy generation, optimise energy storage, and manage the intricate interdependencies in multi-energy systems ensures the operational flexibility of PtX technologies across diverse applications.

Finally, future research must address the gaps in life cycle assessments by incorporating comprehensive environmental and economic sustainability metrics. These assessments will provide a clearer understanding of the long-term viability of PtX technologies, particularly in sectors like heavy transportation, aviation, and industry where decarbonisation is critical.

6.2. Emerging Technologies: Potential Role of Quantum Computing

While much of this review has focused on the transformative impact of ML on PtX technologies, it is also essential to briefly highlight an emerging computational technology that could have a profound influence on the future of PtX systems: Quantum Computing. Quantum computing is emerging as a promising technology capable of solving complex optimisation and simulation problems that challenge classical computing methods. Still being in its infancy, quantum computing excels in handling high-dimensional, non-linear optimisation tasks, which are essential in managing complex energy systems, particularly in large-scale applications such as energy and power systems [99]. The ability of quantum algorithms to optimise processes more efficiently could significantly improve the integration of renewable energy sources and enhance system scalability, areas where traditional methods often fall short [100].

Quantum neural networks (QNN) and other quantum-based approaches are gaining attention for their potential to improve real-time control and decision-making systems. QNNs have shown promise in enhancing decentralised energy systems' ability to respond to fluctuating renewable energy inputs, improving operational flexibility and efficiency [101,102]. The synergy between quantum computing and ML also offers new avenues for optimising energy management systems, enabling faster, more accurate predictions and optimisations in highly dynamic environments [103]. Based on these developments, the application of quantum computing in Power-to-X (PtX) technologies could be transformative, particularly in hard-to-decarbonise sectors.

On the other hand, Quantum computing holds significant potential for advancing the development of catalysts essential for green hydrogen production. Recent studies have explored the potential of quantum simulations to optimise molecular structures and improve catalytic efficiency in such reactions. For instance, quantum spintronic mechanisms have been applied to enhance the efficiency of water-splitting devices through polaron surface states, offering a promising approach to hydrogen generation while minimising energy consumption [104]. Similarly, quantum-enhanced simulations of material properties, such as the spin-orbital coupling in cerium oxide catalysts, have shown substantial improvements in hydrogen yield, reducing the need for expensive catalysts like platinum [105].

While we briefly mentioned the role of quantum computing here due to its critical importance, we acknowledge that this is a subject deserving of independent and detailed study. As quantum computing continues to evolve, its applications in PtX systems are likely to become a significant area of research, with the potential to reshape energy systems and help achieve decarbonisation goals across industrial sectors.

The field of PtX systems is evolving towards a more integrated, dynamic, and resilient approach to energy system management, where machine learning plays a pivotal role. ML enables the optimisation of PtX technologies, making them more adaptable to the complexities of renewable energy integration. With continued advancements, PtX systems, driven by machine learning, are poised to become foundational components of a decentralised and carbon-neutral energy future. By improving energy conversion efficiency, optimising storage, and enhancing operational flexibility, ML is accelerating the transition toward sustainable energy systems that can meet the growing global demand for clean energy while addressing the challenges of intermittent renewable sources.

6.3. Future Directions

Despite the clear advancements, significant gaps remain in ML's application to PtX systems. One of the main limitations is the scalability of ML algorithms, particularly in managing larger-scale PtX operations. Current research focuses primarily on small-to-medium scale systems, and more work is needed to adapt these solutions for industrial-scale applications, especially in the context of large energy storage systems like liquid air energy storage (LAES) and Power-to-Methane.

Moreover, many ML applications are still limited by the availability and quality of real-time operational data. Machine learning models require vast amounts of high-quality data to optimise performance, but many PtX systems suffer from fragmented data sources and inadequate monitoring infrastructure. This impedes the ability of ML algorithms to provide accurate real-time optimisation, limiting their effectiveness in fully autonomous PtX systems.

Additionally, while ML models have been successfully applied to optimise fuel production processes and energy system management, there is a notable lack of comprehensive life cycle assessments (LCA) in existing studies. Without these assessments, the environmental impacts of PtX technologies, including emissions from energy conversion processes, water use, and resource consumption, remain poorly understood. This represents a significant gap in assessing the sustainability of PtX systems.

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To address these limitations, future research should focus on improving the scalability of ML applications in PtX systems. This includes developing more advanced algorithms capable of handling larger datasets and more complex system interactions, especially in the context of multi-energy systems (MES). Machine learning models that can simultaneously optimise energy generation, storage, and consumption across sectors will be essential for advancing PtX processes.

There is also a pressing need for more robust data management frameworks that ensure the availability of high-quality, real-time operational data across PtX systems. This will allow ML models to perform more accurate predictive diagnostics and dynamic optimisation, improving system resilience in fluctuating energy environments.

Furthermore, integrating machine learning with emerging digital technologies such as the Internet of Things (IoT), big data analytics, and cloud-based infrastructure could offer new possibilities for real-time monitoring and optimisation of PtX systems. This approach could significantly improve the operational flexibility and scalability of PtX processes, especially in managing distributed energy resources in decentralised systems.

7. Conclusion

This review has showcased the transformative impact of machine learning on advancing Power-to-X technologies by optimising processes, enhancing operational flexibility, and addressing complex energy storage challenges. ML techniques, including deep learning, reinforcement learning, and data-driven optimisation, have proven crucial in overcoming the intricacies of PtX systems, particularly in dealing with renewable energy intermittency, multi-energy integration, and real-time decision-making.

While significant progress has been made, several challenges remain. Data management, computational demands, and the real-time optimisation of PtX systems still present obstacles that must be addressed. Future research should prioritise the development of more sophisticated ML algorithms capable of handling the large-scale, real-time complexities inherent in PtX technologies. Furthermore, integrating machine learning into multi-energy systems in an effective way will be essential to achieving both operational efficiency and long-term sustainability.

Beyond the current applications of ML, emerging technologies such as quantum computing offer new frontiers for optimisation in PtX. The computational power of quantum systems could further enhance process optimisation, catalyst discovery, and energy system scalability. This represents a critical area for future interdisciplinary research, as the synergy between ML and quantum computing may hold the key to solving the most pressing challenges in decarbonisation and renewable energy integration.

Machine learning will be an indispensable tool in the future of PtX systems, driving innovation in energy conversion, storage, and system flexibility. To fully realise this potential, ongoing advancements in both ML technologies and energy system integration are necessary. Addressing these challenges through interdisciplinary collaboration will accelerate the global transition to a decentralised, carbon-neutral energy future.

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Appendix A

Table A1. Recent review articles that cover subjects in relation with PtX.

Reference	Journal	Category/scope
[106]	International Journal of Hydrogen Energy	hydrogen catalysis and production - Biohydrogen, Machine learning, Nanocatalyst
[107]	International Journal of Hydrogen Energy	hydrogen catalysis and production - Density functional theory, Electrocatalyst, Green hydrogen
[108]	Energy	hydrogen catalysis and production - Analysis and prediction, Hydrogen production, Machine learning
[18]	Fuel	hydrogen catalysis and production - Artificial intelligence, Bibliometric analysis, Deep learning
[14]	International Journal of Hydrogen Energy	hydrogen catalysis and production - Control, Hydrogen, Modeling
[15]	Gaodianya Jishu/High Voltage Engineering	hydrogen catalysis and production - electrolyzer, hydrogen production, model properties
[109]	MRS Bulletin	hydrogen catalysis and production - Autonomous research, Electrochemical synthesis, Energy storage
[110]	International Journal of Hydrogen Energy	hydrogen catalysis and production - Artificial neural networks, Biomass processes, Hydrocarbon pyrolysis
[111]	Applied Sciences (Switzerland)	hydrogen catalysis and production - Alkaline water electrolysis, Hydrogen production technologies, Hydrogen storage methods
[112]	Chemical Engineering Journal	hydrogen catalysis and production - Catalysis, Computational fluid dynamics (CFD), Density functional theory (DFT)
[113]	Journal of Energy Chemistry	hydrogen catalysis and production - Algorithm development, Computational modeling, HER catalyst synthesis
[114]	Environmental Chemistry Letters	hydrogen catalysis and production - Activated carbon, Bioenergy, Hydrogen
[115]	International Journal of Hydrogen Energy	hydrogen catalysis and production - Chemometrics, Data science, DFT
[116]	Electrochemical Energy Reviews	hydrogen catalysis and production - Electrocatalysts, In-situ techniques, Oxygen evolution reaction
[16]	Renewable and Sustainable Energy Reviews	hydrogen catalysis and production - Degradation, Demand response, Dynamic operation
[17]	Energy and AI	hydrogen catalysis and production - AI, Control, Management system
[117]	International Journal of Hydrogen Energy	hydrogen catalysis and production - Computational modeling, Density functional theory, Heterogeneous catalysis
[118]	Matter	hydrogen catalysis and production - carbon utilization, catalysis, cheminformatics
[119]	Advanced Science	photocatalysis for hydrogen production - carbon dioxide reduction, fischer tropsch, material modeling
[120]	Chemical Communications	photocatalysis for hydrogen production -
[121]	Advanced Functional Materials	photocatalysis for hydrogen production - biomass exemplifications, DFT-data driven approach, energy carriers
[122]	Materials Today Catalysis	photocatalysis for hydrogen production - Carbon nitrides, Hydrogen, Photocatalysis
[123]	Chemistry of Materials	photocatalysis for hydrogen production -
[124]c	Journal of Photochemistry and Photobiology C: Photochemistry Reviews	photocatalysis for hydrogen production - Dye-sensitization, Hydrogen generation, Organic and inorganic dyes
[125]	Chemical Engineering Journal	photocatalysis for hydrogen production - Electricity, Hydrogen generation, Photocatalytic fuel cell
[126]	Clean Technologies and Environmental Policy	photocatalysis for hydrogen production - Bibliometric data, Cluster analysis artificial intelligence, Machine learning

[127]	ACS Catalysis	photocatalysis for hydrogen production - CO₂ reduction, machine learning, photoelectrochemistry, halide perovskites
[128]	Nanotechnology	photocatalysis for hydrogen production - Biocatalysis, Multiple exciton generation, Photocatalysis
[129]	Journal of Composites Science	hydrogen storage - Artificial intelligence, Hydrogen storage, Machine learning
[130]	Materials Today Energy	hydrogen storage - Hydrogen storage, Machine learning, Metal organic frameworks
[131]	Journal of Energy Storage	hydrogen storage - Dewarâ€"Kubas interaction, First-principles, Functional groups
[132]	Nano Research	hydrogen storage - model-driven material development processes, nanomaterials, nanotechnology
[133]	Open Research Europe	hydrogen storage - economic requirements, energy transition, porous media
[134]	Progress in Energy	hydrogen storage - adsorption, energy storage, machine learning
[135]	Fuel	hydrogen storage - Electronic structure, First principle calculations, Machine learning
[136]	Chemical Engineering Journal	hydrogen storage - Catalysis, Computational, MOFs
[137]	Renewable and Sustainable Energy Reviews	hydrogen storage - China, Feasibility analysis, Geochemical reactions
[138]	Capillarity	hydrogen storage - lattice boltzmann method, navier-stokes equation, Numerical method
[139]	Coatings	hydrogen storage - HEAs, high-entropy alloys, hydrogen storage
[140]	International Journal of Hydrogen Energy	hydrogen storage - Hydrogen storage, Machine learning, Metal hydrides
[91]	Energy and Fuels	Sustainable Fuel
[141]	Renewable and Sustainable Energy Reviews	Sustainable Fuel - Fischer-Tropsch
[142]	Journal of Energy Chemistry	Sustainable Fuel
[143]	Current Opinion in Green and Sustainable Chemistry	Sustainable Fuel
[144]	Carbon Capture Science and Technology	Sustainable Fuel
[145]	Cailiao Gongcheng/Journal of Materials Engineering	Sustainable Fuel
[19]	Polymers	Envrionmental, economic, strategy, management, and policy - hydrogen storage (tank), nanocomposite(s), nanotubes
[20]	Energy Conversion and Management	Envrionmental, economic, strategy, management, and policy - Economic and environmental impacts, Engineering and theoretical prospects, Hydrogen production
[21]	Energies	Envrionmental, economic, strategy, management, and policy - energy footprint, green hydrogen, green hydrogen guarantees of origin
[146]	Energy and AI	Envrionmental, economic, strategy, management, and policy - Demand-side management, Dynamic power Dispatch, Energy storage
[92]	Advances in Applied Energy	Power-to-Heat - Building energy flexibility, Data-driven, Model predictive control
[22]	Energies	PtX - big data, electrolysis, IoT
[147]	Catalysts	simulation acceleration - non-thermal plasma reactors, plasma, plasma catalysis

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