

Challenges in the Techno-Economic Analysis of the Reverse Water-Gas Shift Reaction

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Abstract

Purpose – Global climate change demands multifaceted solutions, especially in the realm of emerging green technologies. Carbon capture and utilization (CCU) technologies are crucial for reducing emissions in sectors where other alternatives are not economically favorable. In recent years, researchers focused on the catalytic reforming of CO₂ with H₂ to produce chemicals and energy source. One of these researched methods is reverse water-gas shift reaction, which can be a cost-competitive solution for syngas according to previous studies.

Design/methodology/approach – Our goal is to have a deeper understanding of reverse water-gas shift as an alternative way of carbon utilization from an economic perspective. In our research, we utilized literature sources and MS Excel to develop our own model.

Findings – In our study, analysis of literature and the model developed using MS Excel reveal that the RWGS process as a chemical CO₂ conversion route could serve as a sustainable alternative for syngas production, contingent upon the simultaneous presence of multiple factors. However, considering the current TRL of this technology and the anticipated high, yet scalable, maintenance costs, achieving profitability necessitates a significantly large plant scale. Alternatively, profitable operation could be attained through regulatory changes, such as an increase in CO₂ ETS credits.

Since the number of available literatures is highly limited, and the technology has a lower level of TRL, there is a lot of uncertainty in our techno-economic analysis. However, it is clear that for this technology to be profitable, many factors must come together at the same time.

Originality – This is the first empirical work that integrates economic decision-making theory with training transfer mechanisms, incorporating factors that organizations can control to optimize human capital investments. Additionally, establishing supervisor and peer support as contextual variables extends the widely recognized model by Baldwin and Ford.

Keywords: carbon utilization; reverse water gas shift reaction; syngas; techno-economic analysis

Paper type: Research Article

1. Introduction

Global climate change is one of the most pressing challenges of our time, and it demands immediate global action (Bown et al., 2021). The continuous rise in CO₂ levels, which have reached approximately 420 parts per million, underscores the critical need for effective strategies aimed at both reducing and managing these emissions. If left unchecked, these levels will continue to exacerbate the adverse impacts on ecosystems, human health, and the global climate system. In response to this, various approaches have been proposed to mitigate the effects of rising greenhouse gas emissions, among which Carbon Capture and Utilization (CCU) technologies have emerged as one of the most promising solutions (Ekemezie & Digitemie, 2024). These technologies offer a dual benefit: they not only capture CO₂, thereby preventing its release into the atmosphere, but also enable its conversion into valuable products. This innovative approach not only addresses the urgent need for emissions reduction but also aligns with the goals of a circular carbon economy, where CO₂ is viewed as a resource rather than merely a waste product.

The development and scaling of CCU technologies are crucial to achieving meaningful progress in the fight against climate change, as they represent a potential pathway for both mitigating emissions in hard-to-abate sectors and creating economic value from carbon dioxide.

The reverse water-gas shift (RWGS) reaction is a promising technology for CO₂ utilization, producing syngas as a building block for various chemical processes (González-Castaño et al., 2021; Almajed et al.,

2023). While RWGS has attracted significant attention from researchers, there is a need to quantify its net CO₂ consumption and economic feasibility (Bown et al., 2021). Previously published techno-economic assessments reveal that optimal RWGS conditions involve low temperatures and intermediate pressures, balancing capital and operating costs (Portillo et al., 2023). The economic viability of RWGS largely depends on the availability of low-cost, low-carbon hydrogen sources (Bown et al., 2021). However, in the current literature, the reported data shows significant deviation, which presents a challenge in establishing a reliable basis for the accurate modeling of the RWGS process. In addition, there is also a lack of standardization in techno-economic analyses, making it difficult to gather consistent data and compare results across different assessments.

2. Techno-Economic Analysis Framework

Since CCU technologies are at lower technology readiness level and our experience with them is limited, traditional cost-benefit analysis requires significant adjustments. In response to this challenge, techno-economic analysis (TEA) has become a widely adopted approach for assessing the economic feasibility of these technologies. TEA is a widely known and used methodology among both technical and economic experts, and various methodologies exist for its implementation. It offers a comprehensive framework by integrating financial costs, potential revenue streams, environmental impacts, and technological challenges. According to Suleiman and Rosentrater (2018), techno-economic analysis (TEA) is a systematic assessment of economic feasibility aimed at identifying opportunities and risks in projects, considering capital, variable (operational), and fixed costs, as well as benefits (Suleiman & Rosentrater, 2018).

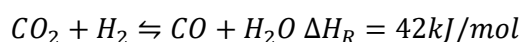
Others define techno-economic analysis as an evaluation of economic feasibility and the impact of parameters most influencing successful deployment (Guerrero et al., 2023). Techno-economic assessment can help determine the technical and economic requirements for the profitability of successful infrastructure development strategies (Koratagere Anantha Kumar & Oughton, 2022). Similarly, TEA can help identify the technical and economic requirements for the profitability of successful strategies (Koratagere Anantha Kumar & Oughton, 2023).

According to Mishra et al., TEA at the research and development scale is an essential step toward the commercialization of any new technology or product as large-scale industrial processes (Kumar Mishra et al., 2023). Meanwhile, Scown and colleagues describe TEA as an empirical, data-driven approach to process design and simulation for estimating capital costs, operational costs, mass balances, and energy balances in a commercial-scale technology (Scown et al., 2021). The simplest approach is described by Horvath and colleagues, who define this analysis as a cost-based technology assessment (Horvath et al., 2018).

This is especially critical for CCU technologies, which typically involve high initial capital investments and significant variations in operational costs. As a result, TEA provides a more nuanced understanding of their long-term economic viability.

2.1 Technical Considerations

One of the research directions explored in recent years is catalytic CO₂ reforming. One pathway for that is RWGS, which is a promising technology. This reaction appears to be a viable solution for CO₂ utilization, as it converts CO₂ into H₂ and CO, producing valuable syngas that can be further transformed into sustainable fuels and chemicals.



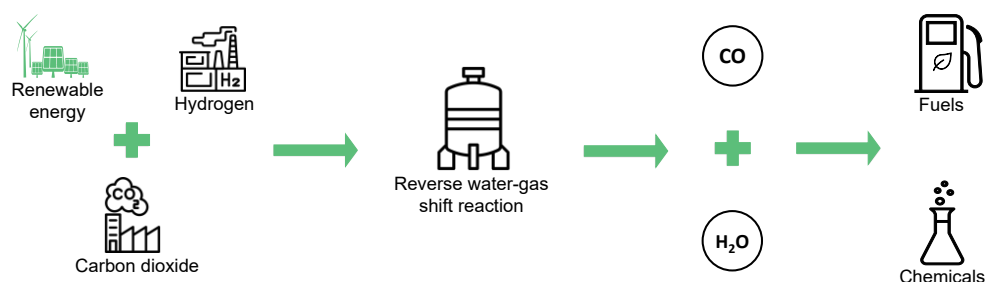


Figure 1 Pathway of reverse water-gas shift

The ratio of CO and H₂ in the syngas produced by the reverse water-gas shift reaction is influenced by several factors. Among others, this ratio is determined by the catalyst used, ratio of H₂ and CO₂ in feed, as well as the reaction temperature and pressure. Since according to thermodynamics CO only becomes the major product above 700 °C, it is important to use a catalyst with high selectivity, capable of operating under this temperature (González-Castaño et al., 2021). The intended form of syngas for further utilization plays a significant role in determining the technical conditions required for the reverse water-gas shift reaction. These conditions must be carefully tailored to ensure the reaction proceeds efficiently and yields the desired product composition.

Numerous studies have been conducted to establish the optimal technical parameters for the process. For instance, Adelung et al. (2021) provided a detailed investigation into the reaction's selectivity, analyzing how varying temperatures and pressures affect the outcome, all while maintaining a consistent H₂/CO₂ ratio in feed. This research contributes valuable insights into understanding the ideal operating conditions for maximizing efficiency and selectivity in the RWGS process. This study had the conclusion that the maximum product output is reachable at 725 °C and 1 bar.

Portillo et al. (2023) provided a comprehensive depiction of the reverse water-gas shift (RWGS) reaction, focusing not only on the catalytic thermodynamics that govern the process but also on the identification of optimal operational conditions. By integrating both the thermodynamic principles and the techno-economic considerations, their study offers a detailed exploration of the reaction's efficiency under various conditions. This dual approach allowed them to determine the most favorable operational parameters, ensuring both technical feasibility and economic viability, ultimately contributing to the broader understanding of RWGS as a key component in carbon capture and utilization technologies.

2.2 Economic Considerations

After deeply understanding all the technological information of RWGS, we studied the available literature to find economic data. In the current literature, there is significant variability in the reported economic data, which presents a challenge in establishing a reliable basis for the accurate modeling of the RWGS process. To enable a comparison of the data available in the literature, we examined the capital investments (CAPEX) and operating costs (OPEX) in relation to capacity. However, as it shows in Table 1., there is significant difference in the available studies. (Table. 1).

Table 1. CAPEX and OPEX in relation to syngas capacity in various studies.

Syngas production capacity (kmol/h)	CAPEX	OPEX	Source
288	\$ 78 260 000	\$ 175 000 000	(Theofanidis et al., 2024)
4 000	\$ 37 470 000	\$ 232 960 000	(Rezaei & Dzuryk, 2019)
22 500	\$ 113 400 000	\$ 1 241 950 000	(Rezaei & Dzuryk, 2019)

23 100	\$ 139 930 000	\$ 559 720 000	(Almajed et al., 2023)
59 342	\$ 378 878 419	\$ 35 120 000	(Zang et al., 2021)

One factor contributing to the significant differences may be variations in production capacity and technical parameters, such as operating temperature and pressure. In studies where syngas was not the final product, we estimated syngas production based on molar masses and the reported data provided in those studies. We then calculated the CAPEX and OPEX specifically for syngas production. This approach allowed us to exclude any additional costs related to further processing or conversion of syngas into other products, providing a clearer and more focused economic analysis.

Upon reviewing the references cited in these studies, it became evident that there is a strong connection between them, as many of the reviewed sources rely on Rezaei's article as a key reference (Fig. 2).

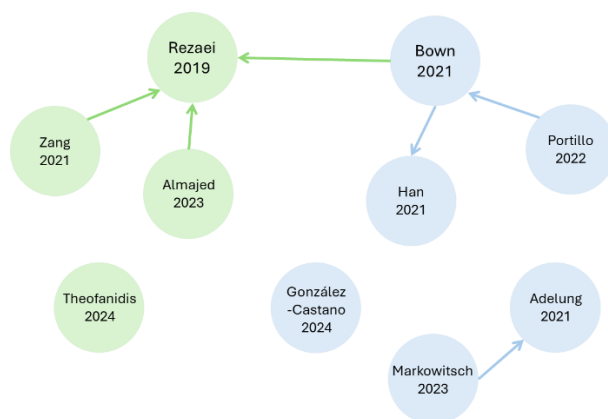


Fig. 2. Connection map of the literature reviewed in this study. Sources where both OPEX and CAPEX data were available are marked in green, while all other referenced literature is marked in blue.

In an effort to broaden our perspective, we conducted an additional search for more independent literature that could provide fresh insights into the economic aspects of the RWGS process (Fig 3.).

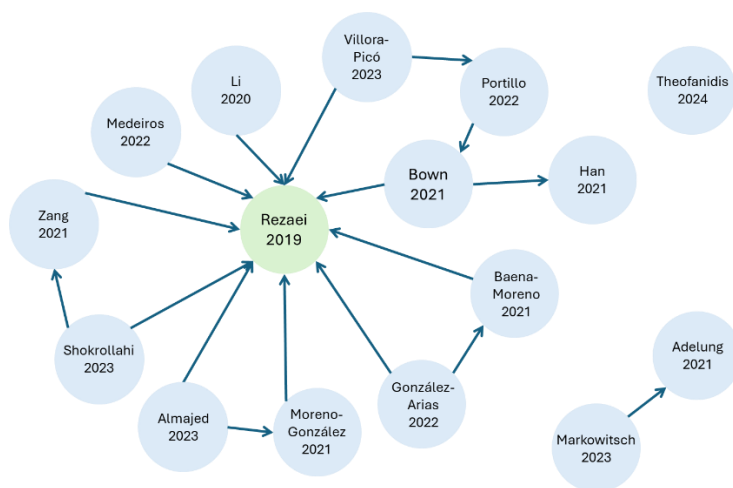


Fig. 3. Results of additional search

Unfortunately, we discovered that a substantial proportion of the articles we found also referred back to Rezaei's work. This frequent citation of the same source, especially regarding CAPEX, highlights the limited availability of diverse, independent data on the economic viability of RWGS. The heavy reliance on a single study creates a bottleneck in the existing literature, further emphasizing the need for new, comprehensive economic analyses to diversify knowledge on this topic.

The cost breakdown of OPEX varies significantly across the available literature, primarily due to differences in the methodologies and the assumptions made regarding operational parameters, such as energy consumption, catalyst use, and maintenance. Some studies include additional costs, like labor, utilities, or infrastructure, while others may focus solely on the core process expenses. These variations create a wide range of OPEX estimates, making direct comparisons between studies challenging.

However, one common conclusion across most of the research is that the largest contributor to the overall operating cost of the RWGS is the cost of hydrogen. (Bown et al., 2021; Adelung et al., 2021). This is largely because hydrogen, especially when sourced from renewable or low-carbon methods like electrolysis, tends to be expensive, accounting for a substantial portion of the total operational expenditures. As a result, the economic feasibility of the RWGS process is heavily dependent on access to affordable hydrogen, and any significant reductions in hydrogen costs could drastically improve the viability of the technology.

Since this reaction operates at high temperatures, the maintenance costs may be higher compared to other carbon capture and utilization (CCU) technologies. This elevated cost is largely due to the wear and tear on equipment, as well as the need for more robust materials that can withstand the extreme conditions.

Previous studies indicate that the operational lifetime of a RWGS plant can range from 10 to 20 years. This relatively long lifespan can help offset some of the initial investment and maintenance costs over time, making the technology more viable in the long-term.

3. Methodology and Data Input

From the available literature, we made our own model to study the feasibility of a plant with 100 000 t/year syngas capacity. Figure 4 represents the scope of boundaries considering the study. The feed is a mixture of H₂:CO₂ with the ratio of 3:1 which is assumed to be available on site already as feedstock. In order for the RWGS reaction to be a net consumer of CO₂, H₂ should be produced from water electrolysis using electricity generated from renewable resources.

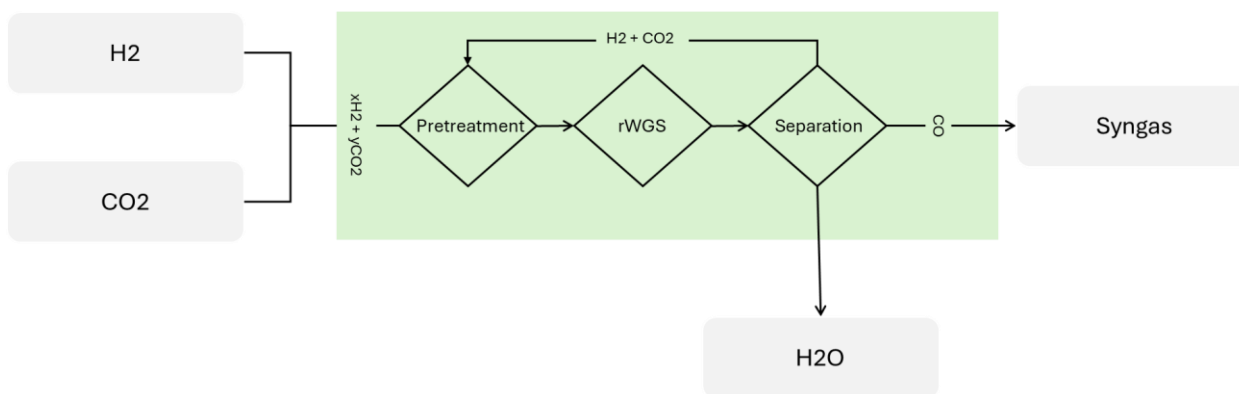


Fig. 4. Technical boundaries of this study

3.1 Technical Considerations

According to several studies, it is shown that for efficient syngas/ CO generation a significant surplus of H₂ is required in the feedstock for the reaction, therefore 3:1 ratio of H₂ to CO₂ is used as feed. Due to its endothermic nature, the reaction favors high temperature, which based on earlier studies is most commonly set to be over 700 °C. Depending on different use cases, pressure can be as high as 3000 kPa. Based on the results of Rezaei & Dzuryk (2019), in this assessment a reference temperature and pressure is

set to 900°C and 410 kPa respectively, in which case the favored reaction is possible with minimal side product formation.

Table 2. Technical Parameters

H2 ratio in feed	0,74	%
CO2 ratio in feed	0,26	%
Temperature	900	°C
Pressure	410	kPa
CO yield	52	%
CO2 conversion	52	%

Furthermore, the reaction is dependent on the use of catalysts, significantly impacting yield and conversion rates. For this study 52% CO₂ conversion rate with a 99,94% selectivity towards CO is assumed, based on the thermodynamic considerations proposed by Rezaei & Dzuryk. As green H₂ is a significant part of the cost breakdown, the model considers the cost of H₂ production via PEM electrolysis, which is based on the assessment of Raya-Imbernon et. al. (2023).

3.2 Economic Analysis

We started the development of our own techno-economic model, based on information from previously presented literature sources to establish a comprehensive framework. Despite making progress in certain areas, we continue to face challenges, particularly when it comes to accurately estimating the CAPEX of the RWGS process.

Based on the previously presented literature review, we attempted to determine the CAPEX of the RWGS process. Given that we found explicit cost calculations only in the studies by Rezaei & Dzuryk (2019) and Theofanidis et al. (2024), we relied on these two sources as the foundation for our analysis. We plotted the reported CAPEX values as a function of plant capacity and subsequently derived a fitted function based on these data points. Using this fitted function, we estimated the CAPEX for our proposed facility.

In the current available literature, we found, that the number of operational days per year range between 315 and 345 days. Therefore, we averaged this to 330 days, equivalent to 7,920 hours of annual operation. The plant's lifespan is commonly determined to be 20 years, according to multiple literature sources (Han, 2021; Markowitsch & Lehner, 2023).

The most significant expense in the process is the cost of hydrogen, which is dependent on electricity prices. Therefore, in our model, the electricity price is the most crucial variable. The hydrogen cost calculation was based on the relationship found in the following article (Raya-Imbernón et al., 2024).

Besides the lack of reliable data on CAPEX of RWGS, our analysis indicates, that our modeled plant is not profitable at the current level; however, it is important to note that the literature presents a significant amount of uncertainty. To ensure the reliability of our analysis, we are conducting a thorough review of the available literature on the CAPEX of SMR. Given the technological similarities between the two processes, examining SMR's capital costs will provide valuable insights and allow us to create more accurate CAPEX estimates for RWGS.

To enhance the reliability of our findings, conducting a sensitivity analysis will be an essential next step for the study. This analysis will help to identify how variations in key parameters affect profitability, thereby offering a clearer understanding of the uncertainties associated with the existing literature. By addressing these uncertainties, we can improve the robustness of our conclusions and better assess the viability of the RWGS technology in practical applications.

4. Conclusion

In our study, we conducted a thorough analysis of existing literature, which indicates that the reverse water-gas shift (RWGS) process holds promise as a sustainable method for CO₂ conversion into syngas. However, this potential hinges on the concurrent fulfillment of several critical factors. Currently, the technology readiness level (TRL) of RWGS is low, and while the maintenance costs are expected to be high, they may be scalable if implemented in sufficiently large plants. It is also clear, that the largest percentage of OPEX will be attributed to the cost of hydrogen, since this reaction is highly hydrogen intensive.

However, there remains considerable uncertainty regarding CAPEX due to the lack of reliable literature and the interconnections present within the available studies. This skews the overall understanding of capital expenditures associated with the RWGS process. To address this uncertainty, further research is needed to provide a more comprehensive and diverse set of data that can accurately reflect the capital costs involved in implementing this technology.

By analyzing SMR's capital costs and understanding how they scale, we hope to draw parallels that can inform our estimates for RWGS. This step will allow us to develop a more reliable and comprehensive techno-economic model for the RWGS process, which is critical for assessing its feasibility and identifying potential cost-saving measures in future deployments.

However, our study indicates that the RWGS process is not profitable at the current level. Achieving profitability in this context will likely necessitate a significant plant scale and low hydrogen cost. Alternatively, the economic viability of RWGS could improve with favorable regulatory changes, such as an increase in CO₂ emissions trading system (ETS) credits, which would provide additional financial incentives for CO₂ conversion technologies.

It is essential to highlight that the existing body of literature on this subject is limited, and the lower TRL adds a layer of uncertainty to our techno-economic analysis. Despite these challenges, it is clear that for the RWGS process to achieve profitability, a variety of conditions must align harmoniously. This includes not only advancements in the technology itself but also supportive regulatory frameworks and evolving market dynamics that favor the integration of CO₂ conversion methods into broader industrial practices. Addressing these factors will be crucial for the successful adoption and commercialization of RWGS as a sustainable syngas production alternative. To further strengthen the reliability of our findings, a sensitivity analysis will be a crucial next step in this research. Such an analysis will provide deeper insights into the impact of key parameter variations on profitability, offering a more comprehensive understanding of the uncertainties present in the existing literature. By systematically addressing these uncertainties, we can enhance the robustness of our conclusions and more accurately evaluate the feasibility of RWGS technology in real-world applications.

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Conflict of interest:

The authors declare no conflict of interest.

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