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Research Article

Optimizing Hydrogenation Production via Recycle Loop in Aspen HYSYS Simulated Water Gas Shift Reaction: Kinetic and Thermodynamic Analysis

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Abstract

Hydrogen production via the water–gas shift (WGS) reaction plays a central role in modern energy systems, where maximizing the conversion of carbon monoxide (CO) into hydrogen (H_2) and carbon dioxide (CO_2) is essential for process efficiency. This study develops a detailed Aspen HYSYS process model to simulate the WGS reaction in an equilibrium reactor, emphasizing process intensification through a recycle loop. The baseline configuration achieves 80.07% CO conversion at 469.6 °C, whereas introducing a recycle stream elevates conversion to 99.90% at a significantly lower reactor temperature of −91.91 °C. This enhancement is accompanied by an increase in hydrogen production from 44.05 kmol/h to 55.01 kmol/h. The recycle stream rich in CO_2 at low temperature functions as an in situ cooling mechanism, shifting the exothermic equilibrium toward greater H_2 formation in accordance with Le Chatelier's principle. This behavior also increases the thermodynamic equilibrium constant, reinforcing the conversion improvement. Kinetic evaluation relies on Gibbs free energy minimization to determine equilibrium compositions, while thermodynamic analysis underscores the dominant influence of temperature on reaction performance. The findings are consistent with trends reported in the literature and carry meaningful industrial implications. By achieving near-complete CO conversion without additional catalysts or membrane technologies, the recycle strategy reduces reliance on downstream purification units such as PSA and enhances overall energy efficiency through process intensification.

Keywords: water-gas shift reaction; hydrogen production; Aspen HYSYS; equilibrium reactor

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1. Introduction

Hydrogen (H_2) is the most abundant element on Earth, primarily found in water and organic compounds. It is the lightest and simplest element, consisting of a single proton and a single electron, and occurs as a colourless, odourless, and highly flammable gas. Hydrogen has a notably high energy density, with a higher heating value of 141.8 MJ/kg and a lower heating value of 120 MJ/kg at 298 K. Because of its versatility, it can be produced from a wide range of resources through diverse feedstocks, production pathways, and technological processes [1].

Producing hydrogen from cost-effective and environmentally sustainable resources is of great importance, as hydrogen is typically regarded as an energy carrier rather than a primary energy source. A variety of processes are employed to generate hydrogen, with steam reforming being one of the most widely used methods for large-scale production. In the steam reforming (SR) process, hydrocarbons react with steam in the presence of a catalyst, yielding hydrogen along with carbon oxides [2,3].

To reduce the concentration of undesirable carbon monoxide (CO) in syngas during steam

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reforming while minimizing hydrogen loss, several strategies can be employed, among which the water–gas shift (WGS) reaction is particularly significant. The WGS reaction has received extensive attention due to its central role in converting CO into additional hydrogen. In this process, CO reacts with water to yield hydrogen and carbon dioxide, thereby facilitating CO_2 removal and enabling the production of high-purity hydrogen.

$$CO + H_2O \rightleftharpoons H_2 + CO_2 \; \Delta H°_{298K} = -41.1 \text{ kJ/mol} \quad (1)$$

The WGS reaction is reversible and governed by equilibrium, and it is widely recognized as a crucial step in hydrogen production from carbon monoxide and water. Since the reaction is moderately exothermic ($\Delta H°_{(298K)} = -41.1$ kJ/mol), its efficiency decreases at elevated temperatures. Consequently, lower operating temperatures combined with higher H_2O/CO ratios are required to achieve favorable conversion levels [4].

Babatabar and Saidi [5] comprehensive computational model that integrates ASPEN Plus with sensitivity analysis to predict and optimize hydrogen production from biomass. Their approach employs an integrated system that combines steam gasification with WGS reaction, enabling more accurate performance evaluation and enhanced process optimization. Živković *et al*. [6] proposed and evaluated a novel industrial-scale reactor design for continuous hydrogen production, employing an intensified WGS process. The design integrates CO_2 sorption using calcium oxide with in-reactor hydrogen separation, thereby enhancing overall efficiency and performance. Chumanee and Nachai [7] investigated strategies to improve the efficiency of the water–gas shift (WGS) reaction by incorporating praseodymium and rhenium into a Co/CeO_2 catalyst. Olateju *et al*. [8] presented a conceptual HYSYS flowsheet for hydrogen production via the WGS reaction. However, the reliance on an equilibrium-based model introduces a technical limitation, which also highlights an opportunity to enhance hydrogen conversion through process-intensification strategies.

A notable gap exists in catalyst-free strategies for enhancing WGS conversion under industrially relevant conditions. This study addresses that gap by introducing a process-intensification approach that incorporates a recycle loop, redirecting the outlet stream from the bottom separator back to the reactor inlet. Through this recirculation, hydrogen conversion can be improved without the need for additional catalysts or costly membrane technologies. The novelty lies in coupling upstream syngas conditioning with reactor staging and dynamic operation, with performance validated through Aspen HYSYS optimization.

2. Methods

The process model for hydrogen production via the water-gas shift reaction was developed and simulated using Aspen HYSYS. In this study, the Peng–Robinson Stryjek–Vera (PRSV) fluid package was selected to represent the thermodynamic behavior of the CO–H_2O–CO_2–H_2 system throughout the simulation. The process employed two fresh feed streams, namely carbon monoxide and steam, which were introduced into a mixer before entering the reactor. The reactor was modeled as an equilibrium type, where the reaction extent was determined based on Gibbs free energy minimization. This approach enabled the calculation of the equilibrium constant and the resulting conversion. After leaving the reactor, the product stream was cooled in a heat exchanger to condense water and heavier components before being routed to a separator. The separator divided the mixture into a hydrogen-rich vapor stream at the top and a liquid-rich stream at the bottom containing unreacted CO, water, and carbon dioxide.

To enhance overall process performance, an additional modification was introduced in the form of a recycle stream. Unlike the base model, where the separator's bottom stream was treated as waste, the modified configuration redirected this stream back to the mixer. The recycle loop was implemented using the recycle block in HYSYS, allowing the software to perform iterative calculations until convergence was achieved for flow rate, temperature, and composition. The recycle stream, consisting primarily of water and unreacted CO, was combined with fresh CO and steam feeds in the mixer. This configuration enabled unreacted CO to undergo multiple passes through the reactor, thereby increasing effective conversion and reducing the requirement for fresh feed.

The flowsheet therefore consisted of a mixer, an equilibrium reactor, a cooler, a separator, a heater, and a recycle loop connected from the separator's bottom stream back to the mixer. The reactor received a combined feed of both fresh and recycled materials, while the separator continued to deliver a hydrogen-rich product through its top stream. The hydrogen product stream was then heated in the final heat exchanger to meet the specified outlet conditions. With the addition of the recycle stream, the process was optimized by examining changes in conversion, hydrogen production rate, and energy requirements. The updated flowsheet demonstrated improved utilization of reactants and enhanced hydrogen yield without altering the main process equipment arrangement.

The reaction in Equation (1), commonly referred to as the water-gas shift reaction, plays a crucial role in the chemical industry, particularly in the large-scale production of hydrogen. In this process, carbon monoxide reacts with steam to yield carbon dioxide and hydrogen. As an equilibrium reaction, it can proceed either toward product formation or revert to the reactants, depending on operating conditions such as temperature and pressure. The direction and extent of this equilibrium are governed by thermodynamics, expressed through the relationship in Equation (2) [9], which connects the equilibrium constant to the Gibbs free energy change of the reaction. A negative ΔG indicates that the reaction proceeds spontaneously toward the products, resulting in a large equilibrium constant, whereas a positive ΔG signifies a non-spontaneous tendency, favoring the reactants. Together, these two equations provide complementary insights: the first outlines the chemical transformation itself, while the second explains the energetic stability and equilibrium position of the system. Together, these two equations provide complementary insights: the first outlines the chemical transformation itself, while the second explains the energetic stability and equilibrium position of the system [8,9].

$$\ln K_{eq} = \frac{\Delta G_{reaction}}{RT} \quad (2)$$

3. Results and Discussion

3.1 Process Design and Optimization

At this stage, the basic model (Figure 1) was modified by introducing a recycle stream from the bottom of the separator back to the reactor inlet (Figure 2). This addition significantly altered the operating conditions, particularly affecting the total feed flow rate and the gas composition entering the reactor. The increased flow rate led to a reduction in residence time per pass, thereby decreasing the per-pass conversion. However, the recycle loop allows unreacted species to return to the reactor, providing additional opportunities for reaction in the subsequent passes. This mechanism aligns with the findings reported by Brübach *et al.* [10], where a once-through configuration achieved only ~40% conversion. Introducing a recycle ratio of R = 1 increased the overall conversion to ~60%, and further to approximately 80% at R = 4, despite the reduction in per-pass conversion due to shorter residence time. A comparison of the gas compositions before and after the inclusion of the recycle stream is presented in Tables 1 and 2 (basic and modified process, respectively).

The optimized process developed in this study exhibits a similar trend. The recycle stream returns unreacted CO to the reactor, thereby increasing the cumulative number of reactants

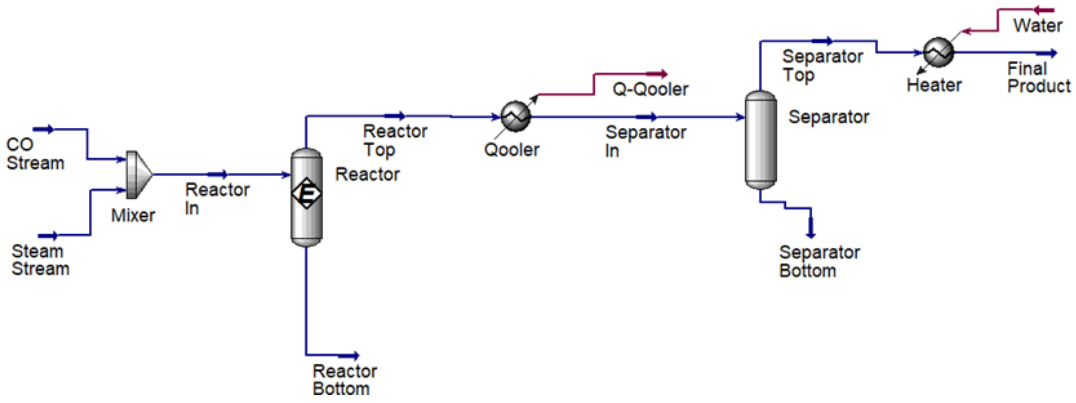

Figure 1. Aspen HYSYS process simulation of water gas shift process without recycles (basic design).

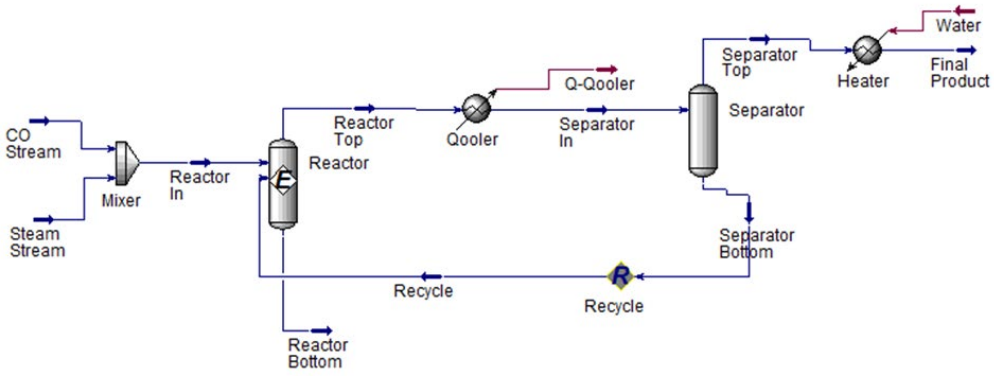

Figure 2. Modified Aspen HYSYS process simulation of water gas shift process with recycles.

undergoing conversion and resulting in a total conversion approaching 100%, specifically 99.90%. In this configuration, the recycle stream does not carry H_2O, so the Steam-to-Carbon ratio remains constant. Thus, the increase in conversion does not originate from changes in feed stoichiometry, but rather from the greater number of gas cycles passing through the reactor. Additionally, the elevated CO_2 fraction introduced via recycling shifts the thermodynamic conditions toward a more favorable state for achieving higher overall conversion. This behavior aligns with the findings of Brübach *et al.* [9], who demonstrated that gas recycling enhances overall conversion once the system reaches steady state. Therefore, the implementing of a recycle stream clearly provides a substantial improvement in total conversion compared to the basic process without recycling.

3.2. Kinetic and Thermodynamic Analysis

3.2.1 Kinetic Consideration

From a kinetic perspective, the water–gas shift (WGS) reaction exhibits a mechanism that is strongly depends on the catalyst employed. In general, the reaction rate follows Arrhenius behavior, increasing with temperature, but its effectiveness is highly influenced by the catalyst type. The WGS reaction operates in two main regimes: the High-Temperature Shift (HTS) and the Low-Temperature Shift (LTS). Fe–Cr catalysts function through a redox mechanism that is active in the HTS region, whereas Cu–Zn–Al catalysts operate predominantly via an associative mechanism in the LTS region [10].

However, it is important to note that the reactor model used in this simulation is an equilibrium reactor, which does not incorporate kinetic expressions but instead determines the outlet composition using Gibbs free energy minimization. The Gibbs minimization method is applied to obtain the equilibrium composition of a reaction system by identifying the condition at which the total Gibbs free energy reaches its minimum value. This approach does not require specifying detailed reaction equations; it only requires listing all possible species in the system along with operating conditions such as temperature and pressure. The algorithm then iteratively calculates the distribution of species until the thermodynamically most stable composition is achieved. The resulting equilibrium composition can subsequently be used to determine the conversion, selectivity, and yield under equilibrium conditions [11].

Table 1. Main stream composition before recycle of basic process.

Process Stream	Composition (%mole)			
	CO	H_2O	CO_2	H_2
CO Stream	1.0000	0.0000	0.0000	0.0000
Steam Stream	0.0000	1.0000	0.0000	0.0000
Reactor In	0.4400	0.5600	0.0000	0.0000
Reactor Top	0.0877	0.2077	0.3523	0.3524
Reactor Bottom	0.0877	0.2077	0.3523	0.3524
Separator In	0.0877	0.2077	0.3523	0.3524
Separator Top	0.0000	0.0000	0.0000	1.0000
Separator Bottom	0.1354	0.3207	0.5440	0.0000
Final Product	0.0000	0.0000	0.0000	1.0000

Table 2. Main stream composition with recycle of modified process.

Process Stream	Composition (%mole)			
	CO	H_2O	CO_2	H_2
CO Stream	1.0000	0.0000	0.0000	0.0000
Steam Stream	0.0000	1.0000	0.0000	0.0000
Reactor In	0.4400	0.5600	0.0000	0.0000
Reactor Top	0.0003	0.0000	0.6992	0.3005
Reactor Bottom	0.0000	0.1907	0.8093	0.0000
Separator In	0.0003	0.0000	0.6992	0.3005
Separator Top	0.0000	0.0000	0.0000	1.0000
Separator Bottom	0.0004	0.0000	0.9996	0.0000
Final Product	0.0000	0.0000	0.0000	1.0000
Recycle CO	0.0004	0.0000	0.9996	0.0000

3.2.2. Thermodynamic Consideration

The water gas shift reaction is expressed in Equation (1). The Water Gas Shift (WGS) reaction is exothermic, and its equilibrium position is highly sensitive to temperature variations. A decrease in temperature increases the equilibrium constant (K_{eq}), thereby shifting the reaction toward the formation of CO_2 and H_2, whereas an increase in temperature drives the equilibrium back toward the reactants [12].

In the optimized (modified) process, the reactor temperature is substantially lower than in the base case. Aspen data indicate that the value of K_{eq} rises sharply, from 6.8149 in the basic (unmodified) process to 3.822×10^9 after optimization. This pronounced increase in Keq reflects conditions that strongly favor near-complete CO conversion. Overall, thermodynamic factors represent the dominant contribution constitute the dominant contribution to the conversion improvement observed in the optimized model.

3.3. Comparison of Optimization Results with the Basic (Unmodified) Process

The comparison between the basic (unmodified) process and the optimized (modified) process is presented in Table 3. The results in Table 3 clearly demonstrate a substantial enhancement in CO conversion, rising from 80.07% in the basic process to 99.90% in the optimized process. This near-complete conversion indicates that the optimized operating conditions have successfully approached the thermodynamic equilibrium limit. In the basic process, the conversion of approximately 80% is consistent with values typically reported for non-optimized water–gas shift (WGS) operations, as noted by Olateju *et al.* [8]. By contrast, the achievement of 99.90% conversion reflects the strong influence of reduced operating temperature, which significantly increases the equilibrium constant in accordance with the exothermic nature of the WGS reaction. The relationship between temperature and equilibrium is described by Moe [13]:

$$K_p = \exp\left(\frac{4577.8}{T} - 4.33\right) \quad (2)$$

where K_p is the equilibrium constant and T is the temperature in Kelvin. This equation shows that K_p increases exponentially when temperature decreases, a characteristic behavior of exothermic reactions. The resulting equilibrium shift is evident in the increase in hydrogen production from 44.05 kmol/h to 55.01 kmol/h, representing a 24.9% improvement, even though the total molar feed rises due to the incorporation of a recycle stream.

Figure 3 illustrates the mole fraction profiles at the reactor outlet with and without recycle. A

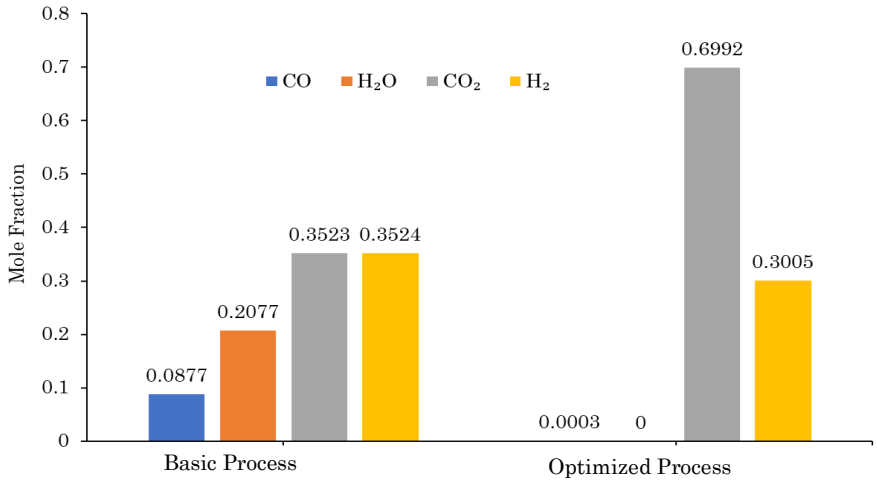

Figure 3. Mole fraction profiles at reactor outlet of the basic (unmodified) process and the optimized (modified) process.

Table 3. Comparison of the basic (unmodified) process and the optimized (modified) process.

Parameter	Basic (unmodified) process	Optimized (modified) process
CO Conversion (%)	80.07	99.90
Total Molar Feed (kmol/h)	125	187.7
H_2 Product (kmol/h)	44.05	55.01
Reactor Outlet Temperature (°C)	469.6	-91.91

pronounced reduction in the CO mole fraction is observed, decreasing from 0.0877 before recycling to just 0.0003 after recycling. This is accompanied by a marked increase in the CO_2 mole fraction from 0.3523 to 0.6992, while the H_2 mole fraction shifts from 0.3524 to 0.3005 after recycling. These compositional changes confirm that the WGS reaction is strongly driven toward the product side when recycling is applied, consistent with the increase in the equilibrium constant at lower operating temperatures. As a result, CO conversion approaches its thermodynamic limit with high efficiency, maximizing hydrogen yield while minimizing residual CO in the product stream.

3.4 Optimization Analysis of Recycle Effect

The near complete conversion (99.90%) achieved in the optimized (modified) process is primarily driven by the implementation of the recycle stream, which function as an internal cooling system (in situ cooling). The recycle stream returning to the reactor inlet is rich in CO_2 and has already been cooled downstream; when mixed with the fresh feed, it lowers the reactor inlet temperature without requiring an external heat exchanger. This reduction in temperature directly enhances the equilibrium constant (K), as described by the Moe equation, thereby shifting the exothermic WGS reaction toward the products in accordance with Le Chatelier's principle [14]. Thermodynamically, the WGS equilibrium constant (K) is defined by:

$$K = \frac{P_{H_2} \cdot P_{CO_2}}{P_{CO} \cdot P_{H_2O}} \quad (6)$$

where P denotes the partial pressure of each gas. At lower temperatures, the value of K increases exponentially, enabling the system to achieve higher equilibrium conversions.

Although a recycle stream dominated by CO_2 (mole fraction ≈ 0.9996 as shown in Table 4) might theoretically inhibit the forward reaction by increasing the partial pressure of the product, the cooling effect produced by recycling is far more significant than the inhibitory influence of elevated P_{CO2}. A temperature decreases of 50–100 °C can increase K_p by a factor of 2–5 according to the Moe equation, whereas the increase in P_{CO2} due to recycling contributes only linearly in the equilibrium expression. The optimized recycle ratio (0.50 split fraction) ensures that the CO_2 concentration at the reactor inlet does remains controlled, maintaining conditions favorable for high conversion. Dehimi *et al.* [13], in their microkinetic study, showed that at low temperatures (300–400 °C), the surface coverage of intermediate species such as OH and HCOO increases, indicating that the forward reaction rate remains high even when the partial pressure of CO_2 is elevated. Thus, the recycle stream serves as a highly effective temperature-control mechanism and represents a direct application of process intensification, integrating internal cooling, equilibrium-shifting behavior, and energy-efficiency improvements into a single system [15] (Figure 4).

The CO conversion of 99.90% achieved in the optimized (modified) process is consistent with

Table 4. Composition, temperature and molar flow of Recycle Stream.

Parameter	Value
CO (%mole)	0.0004
CO_2 (%mole)	0.9996
H_2O (%mole)	-
H_2 (%mole)	-
Temperature (°C)	-271.1
Molar Flow (kmol/h)	131.5

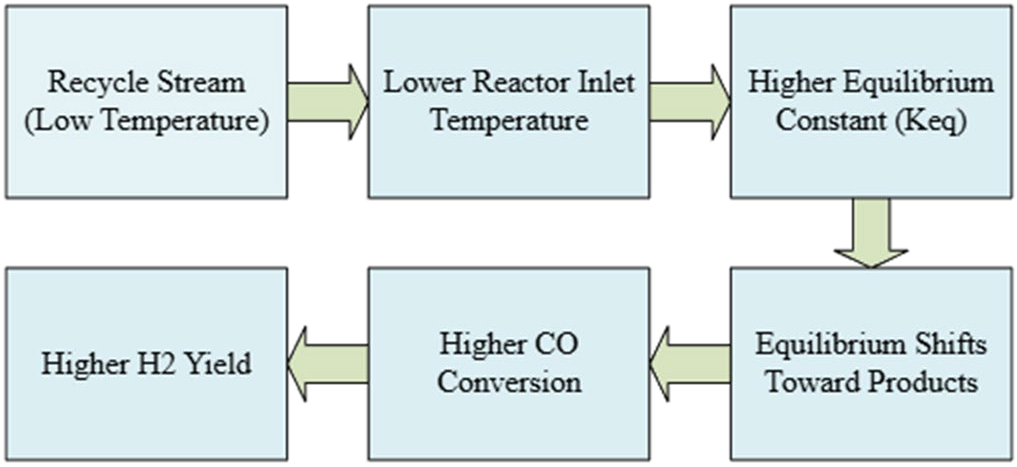

Figure 4. Effect analysis of recycle implementation on WGS reactor performance.

several literature reports. Al Zakwani *et al.* [16] reported CO conversions exceeding 95% in WGS systems operating at 270 °C and 1 bar; Dehimi *et al.* [13] found that CO conversion may reach 91% at 340 °C and approach equilibrium values (>99%) at lower temperatures with high steam to carbon ratios; while Khoshnoudi & Akay [15] achieved 92.8% CO conversion at 300 °C. The increase in CO conversion from 80.07% to 99.90% carries significant implications: the extremely low CO concentration (0.03 mol%) meets the stringent specifications for PEM fuel-cell applications, which require CO levels <10 ppm, thereby reducing or eliminating the need for downstream purification units such as PSA. Moreover, the 24.9% increase in H_2 yield (from 44.05 to 55.01 kmol/h) demonstrates that more hydrogen can be produced from the same amount of feedstock, while the use of recycle as an internal cooling mechanism reduces external cooling requirements, aligning with process-intensification strategies for energy efficiency. In summary, the synergy between lowering the operating temperature through recycling and increasing the equilibrium constant K_p explains why the optimized (modified) process achieves CO conversion as high as 99.90%. This confirms that recycle-based optimization is a highly effective strategy for maximizing conversion in WGS reactors while simultaneously delivering energy-efficiency benefits and superior product quality.

4. Conclusion

Recycling the separator bottom stream to the reactor inlet intensifies the water-gas shift process by providing both in situ cooling and reactant recovery, increasing CO conversion from 80.07% to 99.90% without altering the steam-to-carbon ratio. The substantial rise in the equilibrium constant at the much lower operating temperature makes thermodynamics the primary driver of this improvement, while repeated passes of unreacted CO through the reactor enhance overall feed utilization. This configuration not only raises hydrogen production by roughly 25% but also reduces CO concentrations toward fuel-cell-grade levels, demonstrating that thoughtful process integration can rival or even replace costly catalytic or membrane-based upgrades in WGS systems.

CRedit Author Statement

Author Contributions: Christopher Beryl Nugraha Adi: Conceptualization, Methodology, Simulation and formal analysis, Writing – original draft, Writing – review & editing. Thania Nurjulianti Agus: Data analysis, Validation, Writing – original draft, Writing – review & editing. Muhammad Ridho: Methodology, Process description, Writing – original draft, Writing – review & editing. Virnanda Namia Leonica: Conceptualization support, Data interpretation, Writing – original draft, Writing – review & editing. Naurah Dwicalista Hanifah: Literature study, Data curation, Writing – original draft, Writing – review & editing. All authors have read and agreed to the published version of the manuscript.

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