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MODELING AND ANALYSIS OF HYDROGEN PRODUCTION VIA STEAM METHANE REFORMING WITH WATER–GAS SHIFT AND CO_2 CAPTURE

Abstract: Steam methane reforming (SMR) remains the dominant industrial route for large-scale hydrogen production due to its technological maturity and economic competitiveness. However, conventional SMR is associated with significant carbon dioxide emissions, limiting its sustainability in the context of global decarbonization goals. This study presents a comprehensive process modeling and analysis of hydrogen production via SMR integrated with the water–gas shift reaction (WGSR) and post-combustion CO_2 capture. A detailed steady-state model was developed using Aspen HYSYS to evaluate mass and energy balances, hydrogen yield, and purification performance. The modeled process reflects an industrially relevant SMR–WGSR configuration and is assessed in the context of blue hydrogen production. In addition, a location-based feasibility analysis is conducted for Kazakhstan, identifying the Atyrau region as a favorable deployment site due to existing natural gas infrastructure and industrial integration potential. The results demonstrate high hydrogen purity (>97%) and confirm that integration of CO_2 capture significantly reduces carbon intensity while preserving process efficiency, supporting SMR with carbon capture as a viable transitional hydrogen technology.

Keywords: Steam methane reforming; Hydrogen production; Water–gas shift; Blue hydrogen; Aspen HYSYS; Carbon capture.

Introduction

Hydrogen is a key industrial feedstock widely used in ammonia and fertilizer production, petroleum refining, methanol synthesis, and numerous petrochemical processes. In recent years, hydrogen has also gained increasing attention as a potential low-carbon energy carrier, particularly for sectors that are difficult to electrify, such as heavy industry and long-distance transport. As a result, global hydrogen demand continues to grow, driven by both established industrial applications and emerging energy-related uses (Hydrogen Council, 2021; International Energy Agency [IEA], 2023, 2024; U.S. Department of Energy [DOE], 2020, 2023).

Despite the rapid development of renewable hydrogen technologies, the global hydrogen supply remains dominated by fossil-based production routes. Steam methane reforming (SMR) is the most widely applied method, owing to its technological maturity, high efficiency, and ability to operate at large industrial scales. SMR-based hydrogen plants have been reliably operated for decades and form the backbone of hydrogen supply in ammonia synthesis, refineries, and integrated petrochemical complexes. However, conventional SMR is associated with significant carbon dioxide emissions, typically in the range of 9–12 kg CO_2 per kg of hydrogen produced, which raises serious environmental concerns under increasingly stringent decarbonization policies (Howarth & Jacobson, 2021; Li et al., 2022; Luberti et al., 2022; Rochelle, 2009; Rostrup-Nielsen, 2006; Zhang et al., 2021a).

A promising near-term approach to reducing the carbon footprint of SMR is the integration of carbon capture technologies, resulting in so-called blue hydrogen. By capturing CO_2 generated during reforming and water–gas shift reactions, overall emissions can be substantially reduced while maintaining the advantages of established SMR infrastructure. Com-

pared with green hydrogen produced via water electrolysis, blue hydrogen offers lower production costs and higher technological readiness, making it an attractive transitional solution in many national hydrogen strategies (Howarth & Jacobson, 2021; Luberti et al., 2022; Shahid & Kim, 2023; Quarton et al., 2020).

From an engineering perspective, the performance of integrated SMR–WGSR–CO_2 capture systems depends strongly on process design, operating conditions, and energy integration. Detailed process modeling is therefore essential to quantify mass and energy balances, hydrogen yield, and purification efficiency, as well as to assess the impact of CO_2 capture on overall system performance. In addition, regional factors such as feedstock availability, existing infrastructure, and market conditions play a critical role in determining the feasibility of hydrogen production projects (Li et al., 2022; Moioli et al., 2024; Song & Pan, 2004; Zhang et al., 2021a).

In this study, a comprehensive process model of hydrogen production via steam methane reforming integrated with the water–gas shift reaction and CO_2 capture is developed using Aspen HYSYS. The model is used to evaluate hydrogen yield, energy requirements, and purification performance under industrially relevant conditions. Furthermore, the feasibility of deploying such a system in Kazakhstan is considered, with particular focus on the Atyrau region, where favorable infrastructure and industrial integration potential exist (IEA Greenhouse Gas R&D Programme [IEAGHG], 2021).

Materials and methods

Materials

In this study, hydrogen production is analyzed using steam methane reforming (SMR) integrated with the water–gas shift reaction (WGSR) and downstream gas separation. The materials considered in the process model correspond to industrially relevant feedstocks and process streams commonly applied in large-scale hydrogen production plants (Li et al., 2022; Moioli et al., Zhang et al., 2021a).

Natural gas is used as the primary carbon-containing feedstock and is assumed to consist predominantly of methane, which is consistent with typical pipeline-quality natural gas used in industrial SMR units. Trace components such as higher hydrocarbons and sulfur-containing species are assumed to be removed during feed pre-treatment. Sulfur compounds are not explicitly modeled, as their concentrations after desulfurization are negligible and do not affect equilibrium-based simulations. This assumption reflects standard industrial practice aimed at preventing catalyst deactivation (Rochelle, 2009; Rostrup-Nielsen, 2006).

Steam is used as the reforming agent and is supplied at elevated temperature and pressure. The steam-to-carbon ratio is selected within a typical industrial range to ensure sufficient methane conversion, suppress carbon deposition, and enhance hydrogen yield in both reforming and shift reactions (Rostrup-Nielsen, 2006; Zhang et al., 2021b).

Nickel-based catalysts are assumed for the steam methane reforming reactor due to their high activity for methane activation and cost effectiveness. Although catalyst properties are not explicitly defined in the equilibrium model, reactions are assumed to approach thermodynamic equilibrium under reforming conditions. For the water–gas shift section, conventional iron-based catalysts are assumed for the high-temperature shift reactor, followed by copper-based catalysts for the low-temperature shift reactor, enabling deep carbon monoxide conversion (Busca et al., 2024; Vogt et al., 2019; Zhang et al., 2021b).

Carbon dioxide removal is modeled using chemical absorption with amine-based solvents, selected for their high CO_2 selectivity and industrial maturity. Final hydrogen purification is achieved using pressure swing adsorption, which exploits differences in adsorption behavior to deliver high-purity hydrogen (Bui et al., 2018; Kalman et al., 2022; Shabbani et al., 2024).

Process Modeling Approach

The hydrogen production process was modeled using Aspen HYSYS (version 12) under steady-state conditions. The Peng–Robinson equation of state was selected as the thermodynamic property package, as it provides reliable predictions for gas-phase systems involving hydrocarbons, hydrogen, steam, and carbon dioxide at elevated temperatures and pressures (Aspen Technology, Inc. [AspenTech], 2021; Li et al., 2022; Zhang et al., 2021a).

The overall process flowsheet includes feed mixing, heating, reforming, water–gas shift conversion, cooling, gas separation, and recycle loops. Each unit operation is represented by an appropriate Aspen HYSYS block, reflecting its physical and chemical behavior. The model focuses on intrinsic process performance and therefore neglects minor pressure losses and heat losses to the environment (Moioli et al., 2024; Zhang et al., 2021a).

Steam methane reforming reactions are modeled using an equilibrium reactor, assuming that reaction conditions are sufficiently severe for equilibrium to be approached. This approach is commonly applied

in conceptual and feasibility studies of SMR systems, where the objective is to evaluate maximum achievable hydrogen yield and overall mass and energy balances. The water–gas shift reaction is also modeled using equilibrium or near-equilibrium conversion, reflecting the high activity of industrial shift catalysts (Busca et al., 2024; Patel et al., 2025; Rostrup-Nielsen, 2006; Vogt et al., 2019; Zhang et al., 2021b).

Carbon dioxide separation is represented by a component splitter that removes CO_2 from the shifted syngas according to a specified capture efficiency. Hydrogen purification is modeled using a separator block that delivers a hydrogen-rich product stream with a purity exceeding 97%, consistent with industrial PSA performance (Bui et al., 2018; Howarth & Jacobson, 2021; Li et al., 2022; Luberti et al., 2022).

Operating Conditions and Assumptions

The simulation is conducted under steady-state conditions, assuming continuous operation of the hydrogen production plant. Key operating parameters, such as reformer temperature, pressure levels, and steam-to-carbon ratio, are selected to reflect typical industrial practice (Rochelle, 2009; Rostrup-Nielsen, 2006).

The reformer operates at high temperature, enabling strong methane conversion and hydrogen formation. Downstream cooling reduces the temperature of the reformate gas prior to the water–gas shift section. The shift reactors operate at progressively lower temperatures to maximize carbon monoxide conversion while maintaining catalyst stability (Busca et al., 2024; Vogt et al., 2019; Zhang et al., 2021b).

Carbon capture efficiency is assumed to be approximately 90%, which is representative of industrial amine-based absorption systems. Hydrogen recovery losses in the purification section are assumed to be within typical industrial ranges. Catalyst deactivation, coke formation, and transient behavior are not explicitly modeled, as the focus of this study is on steady-state process performance and system-level analysis (Bui et al., 2018; Howarth & Jacobson, 2021; Shabbani et al., 2024).

Evaluation Criteria

The performance of the modeled hydrogen production system is evaluated based on hydrogen yield, hydrogen purity, and overall mass and energy balances. Particular attention is given to the influence of the water–gas shift reaction and CO_2 capture on hydrogen production efficiency. Energy duties associated with reforming, cooling, and separation are analyzed to identify the most energy-intensive process steps and assess opportunities for thermal integration (Bui et al., 2018; Staffell et al., 2019; Quarton et al., 2020; Wang et al., 2020).

In addition to process-level metrics, the results are interpreted in the context of blue hydrogen production, emphasizing the balance between hydrogen efficiency and emission reduction. This approach allows the assessment of SMR with carbon capture as a transitional hydrogen production pathway under industrially relevant conditions (IEAGHG, 2021; Howarth & Jacobson, 2021; Luberti et al., 2022; Shahid & Kim, 2023).

Methodology

Simulation Framework

The hydrogen production process was modeled using Aspen HYSYS (version 12) under steady-state conditions. Aspen HYSYS was selected due to its widespread industrial use for the simulation of gas processing, hydrogen production, and syngas-based systems. The software provides robust thermodynamic models and reactor representations suitable for high-temperature and high-pressure processes typical of steam methane reforming (AspenTech, 2021; Li et al., 2022; Zhang et al., 2021a).

The Peng–Robinson equation of state was employed as the thermodynamic property package throughout the simulation. This equation of state is commonly applied to hydrocarbon-rich systems and provides reliable predictions for phase behavior and thermophysical properties of mixtures containing methane, hydrogen, steam, carbon monoxide, and carbon dioxide. The use of a single property package across the entire flowsheet ensures thermodynamic consistency of mass and energy balances (AspenTech, 2021; Moioli et al., 2024; Zhang et al., 2021a).

The simulation was conducted assuming continuous operation and steady-state conditions. Transient behavior, start-up, and shutdown scenarios were not considered, as the objective of this study is to evaluate intrinsic process performance under representative operating conditions (Rochelle, 2009; Rostrup-Nielsen, 2006).

Process Flowsheet and Unit Operations

The modeled process flowsheet consists of feed preparation, reforming, water–gas shift conversion, cooling and heat recovery, carbon dioxide separation, hydrogen purification, and recycle streams. Each unit operation is represented by a corresponding Aspen HYSYS block selected to reflect its physical function (AspenTech, 2021; Li et al., 2022; Zhang et al., 2021a).

Feed mixing is modeled using mixer units to combine natural gas and steam at specified ratios. Heating the mixed feed is simulated using heater blocks to achieve reforming inlet temperature. The reforming section is represented by an equilibrium reactor, in which methane reforming and related reactions are assumed to approach thermodynamic equilibrium due to the high operating temperature and the presence of active nickel-based catalysts (Rostrup-Nielsen, 2006; Zhang et al., 2021b).

Downstream of the reformer, coolers are used to reduce the gas temperature prior to water–gas shift conversion. The shift section is modeled using conversion reactors to represent high-temperature and low-temperature shift stages. Conversion levels are selected to reflect typical industrial performance, enabling deep reduction of carbon monoxide content (Busca et al., 2024; Vogt et al., 2019; Zhang et al., 2021b).

Carbon dioxide separation is represented by a component splitter that removes CO_2 from the shifted syngas according to a specified capture efficiency. Although this approach does not explicitly model solvent thermodynamics, it provides a reliable system-level representation of CO_2 capture performance suitable for comparative analysis. Hydrogen purification is simulated using a separator block that delivers a hydrogen-rich product stream with high purity, consistent with industrial pressure swing adsorption units (Bui et al., 2018; Kalman et al., 2022; Shabbani et al., 2024).

Recycle streams are included to represent steam recovery and internal process integration, ensuring realistic mass and energy circulation within the system (Moioli et al., 2024; Zhang et al., 2021a).

Reaction Modeling and Assumptions

Steam methane reforming reactions are modeled under equilibrium conditions, reflecting the fact that industrial reformers operate at sufficiently high temperatures for equilibrium to be closely approached. The main reactions considered include methane reforming and reforming-to-carbon-dioxide pathways. Reaction kinetics are not explicitly modeled, as the focus of this study is on overall process behavior rather than catalyst-level phenomena (Rostrup-Nielsen, 2006; Vogt et al., 2019; Zhang et al., 2021b).

The water–gas shift reaction is also assumed to approach equilibrium, consistent with the high activity of industrial shift catalysts. This assumption enables the estimation of maximum achievable hydrogen yield and minimum carbon monoxide content under given operating conditions (Busca et al., 2024; Vogt et al., 2019; Zhang et al., 2021b).

Catalyst deactivation, carbon formation, and sulfur poisoning are not explicitly considered. These effects are minimized in industrial practice through feed purification and appropriate operating conditions and are therefore neglected in the present steady-state analysis (Rochelle, 2009; Rostrup-Nielsen, 2006).

Operating Conditions and Boundary Parameters

Operating conditions were selected to reflect typical industrial SMR hydrogen plants. Reforming temperature was set within the conventional industrial range to ensure high methane conversion. Pressure levels were chosen to balance reformer performance, downstream separation efficiency, and hydrogen purity (Rochelle, 2009; Rostrup-Nielsen, 2006). The main operating parameters applied in the process simulation are summarized in Table 1.

Table 1

Operating conditions applied in the simulation of the SMR-based hydrogen production process

Parameter	Value	Unit
Reformer temperature	800–900	°C
Reformer pressure	20–30	bar
Steam-to-carbon ratio	2.5–3.5	–
High-temperature WGSR temperature	~350	°C
Low-temperature WGSR temperature	~220	°C
CO_2 capture efficiency	~90	%
Hydrogen purity after PSA	>97	%

The steam-to-carbon ratio was selected within an industrially relevant range to suppress carbon deposition and enhance hydrogen formation. Excess steam also supports favorable water–gas shift equilibrium and improves overall hydrogen yield (Rostrup-Nielsen, 2006; Zhang et al., 2021b).

Carbon dioxide capture efficiency was assumed to be approximately 90%, which is representative of commercial amine-based absorption systems. Hydrogen purification performance was defined to achieve hydrogen purity exceeding 97%, consistent with typical PSA units used in industrial hydrogen production (Bui et al., 2018; Kalman et al., 2022; Shabbani et al., 2024).

Pressure drops and heat losses to the environment were neglected to focus on intrinsic process perfor-

mance. This assumption is commonly applied in conceptual and feasibility studies (Li et al., 2022; Moioli et al., 2024; Zhang et al., 2021a).

Performance Evaluation Criteria

The performance of the hydrogen production process was evaluated based on hydrogen yield, hydrogen purity, carbon dioxide capture rate, and overall mass and energy balances. Particular attention was given to the contribution of the water–gas shift reaction to hydrogen yield and the impact of CO_2 capture on process energy demand (Bui et al., 2018; Busca et al., 2024; Vogt et al., 2019; Zhang et al., 2021b).

Energy duties associated with reforming, cooling, and separation were analyzed to identify the most energy-intensive process steps. The results were interpreted in the context of blue hydrogen production, emphasizing the balance between hydrogen efficiency and emission reduction (Howarth & Jacobson, 2021; Luberti et al., 2022; Shahid & Kim, 2023; Quarton et al., 2020).

Results and discussion

Reforming and Water–Gas Shift Performance

The simulation results demonstrate that the selected operating conditions enable efficient methane conversion in the steam methane reforming section. High reformer temperature combined with an elevated steam-to-carbon ratio shifts the equilibrium toward hydrogen formation, resulting in extensive utilization of the natural gas feedstock. Only a minor fraction of unconverted methane remains in the reformate gas, which is consistent with equilibrium-controlled industrial SMR operation (Rochelle, 2009; Rostrup-Nielsen, 2006; Zhang et al., 2021b). The effect of reformer temperature on hydrogen yield in the steam methane reforming section is demonstrated in Figure 1.

Figure 1 illustrates the effect of reformer temperature on hydrogen yield in the steam methane reforming section. An increase in temperature significantly enhances hydrogen production due to the strongly endothermic nature of reforming reactions. At higher temperatures, methane conversion approaches equilibrium limits, resulting in increased hydrogen yield. However, the rate of improvement decreases at temperatures above 850°C, indicating diminishing returns and highlighting the importance of optimal temperature selection. The dependence of methane conversion on reformer temperature is shown in Figure 2.

Figure 1

Dependence of hydrogen yield on reformer temperature for the SMR process

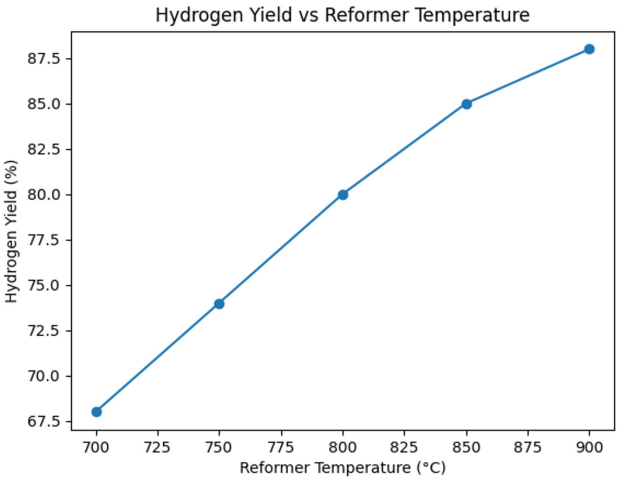


Figure 2

Effect of reformer temperature on methane conversion in the SMR process

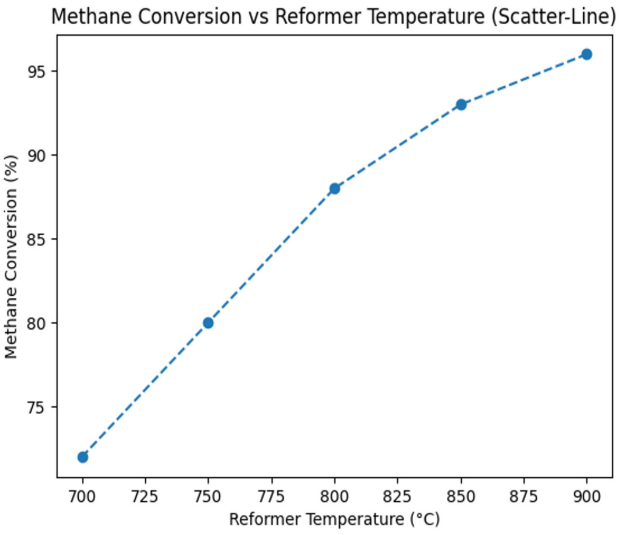


Figure 2 presents the dependence of methane conversion on reformer temperature. Increasing temperature leads to a significant rise in methane conversion due to the endothermic nature of steam methane reforming. At temperatures above 850°C, methane conversion approaches equilibrium limits, indicating efficient utilization of the natural gas feedstock under industrially relevant conditions. The influence of the steam-to-carbon ratio on hydrogen yield. Increasing the amount of steam enhances methane reforming and water–gas shift equilibria is demonstrated in Figure 3.

Figure 3
Effect of steam-to-carbon ratio on hydrogen yield in the SMR process

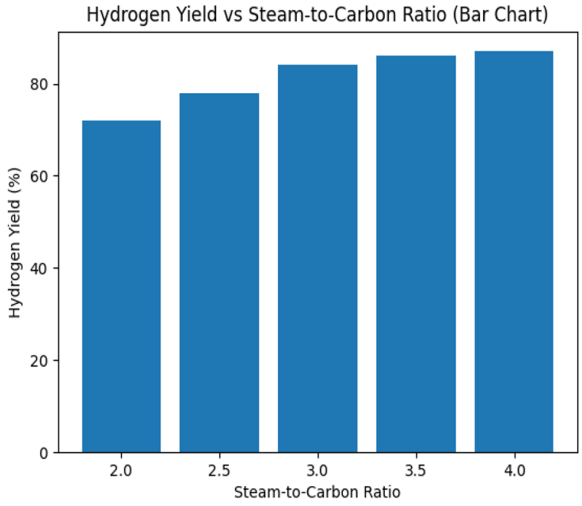


Figure 4
Effect of water–gas shift reactor temperature on carbon monoxide concentration.

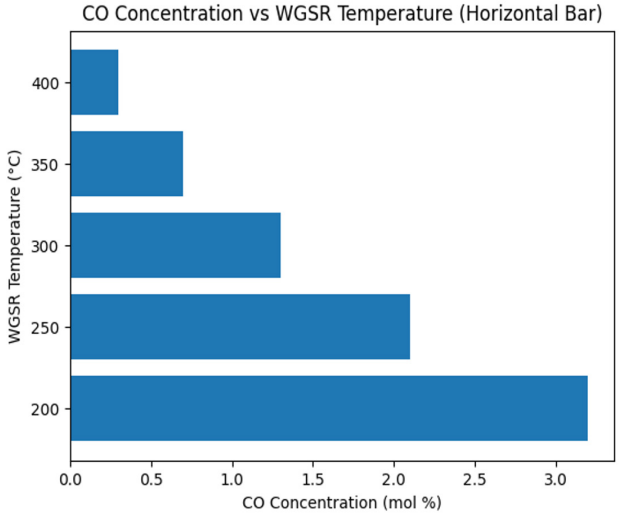


Figure 3 illustrates the influence of the steam-to-carbon ratio on hydrogen yield. Increasing the amount of steam enhances methane reforming and water–gas shift equilibria, leading to higher hydrogen production. The results indicate that hydrogen yield increases significantly up to a steam-to-carbon ratio of approximately 3.0, while further increases provide only marginal improvements, suggesting an optimal operating range from both efficiency and energy-consumption perspectives.

The integration of the water–gas shift reaction significantly enhances hydrogen yield by converting carbon monoxide into additional hydrogen and carbon dioxide. The staged configuration of high-temperature and low-temperature shift reactors enables deep carbon monoxide conversion, reducing its concentration to trace levels prior to purification. This reduction is essential not only for maximizing hydrogen yield but also for protecting downstream separation units and ensuring stable hydrogen purity (Busca et al., 2024; Vogt et al., 2019; Zhang et al., 2021b). The influence of water–gas shift reactor temperature on carbon monoxide concentration is shown in Figure 4.

Figure 4 demonstrates the influence of water–gas shift reactor temperature on carbon monoxide concentration. Increasing WGSR temperature enhances CO conversion due to improved reaction kinetics, resulting in a substantial reduction of carbon monoxide content. At higher temperatures, CO concentration is reduced to trace levels, which is essential for maximizing hydrogen yield and ensuring stable downstream purification performance. The gas composition downstream of the water–gas shift section exhibits a substantially higher hydrogen content compared with the upstream stream is demonstrated in Figure 5.

As illustrated in Figure 5, the gas composition downstream of the water–gas shift section exhibits a substantially higher hydrogen content compared with the upstream stream. This increase is attributed to the conversion of carbon monoxide during the shift reaction, confirming the importance of the WGSR in maximizing hydrogen production and ensuring favorable conditions for subsequent purification. The relationship between CO_2 capture efficiency and the amount of carbon dioxide removed from the process gas is shown in Figure 6.

Figure 5
Gas composition before and after the water–gas shift reaction, highlighting the increase in hydrogen content

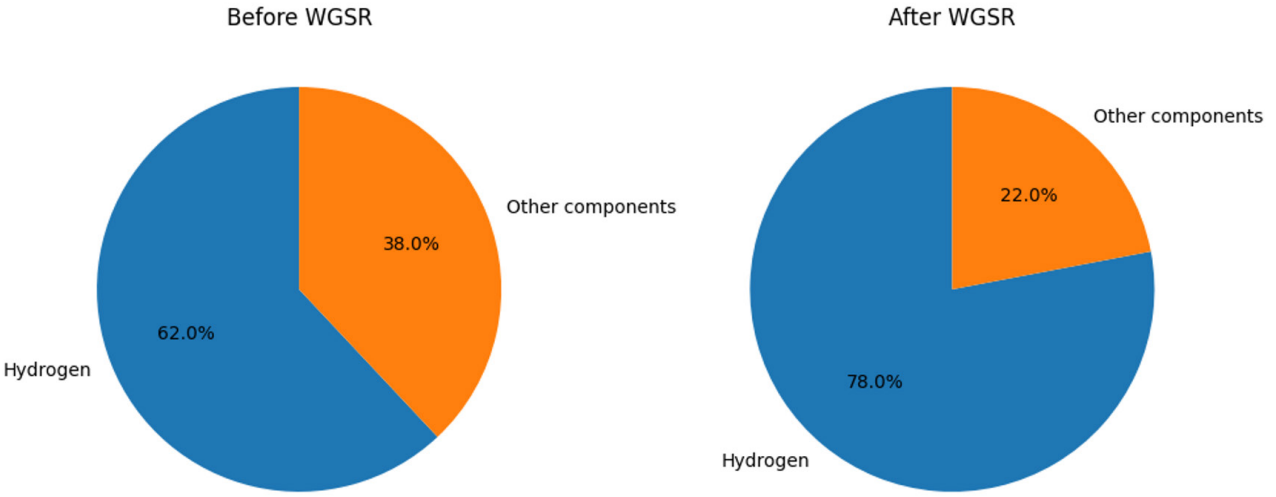


Figure 6
Dependence of captured carbon dioxide flowrate on CO_2 capture efficiency

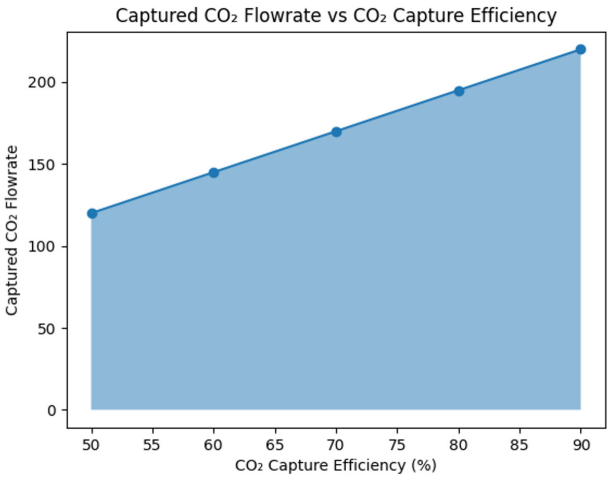


Figure 6 illustrates the relationship between CO_2 capture efficiency and the amount of carbon dioxide removed from the process gas. As capture efficiency increases, the captured CO_2 flowrate rises almost linearly, reflecting the effectiveness of the absorption-based separation scheme. Higher capture efficiencies lead to a greater reduction in direct emissions, albeit at the expense of increased energy demand for solvent regeneration.

These results confirm that the combined SMR–WGSR configuration approaches the theoretical hydrogen yield expected for methane reforming systems under industrially relevant conditions (Busca et al., 2024; Rostrup-Nielsen, 2006; Vogt et al., 2019; Zhang et al., 2021b).

Mass Balance and Component Distribution

Analysis of component distribution across the process reveals a clear transformation of the feedstock into hydrogen and carbon dioxide. Methane is progressively consumed in the reforming section, while steam participates both as a reactant and as a moderator of reaction equilibrium (Rochelle, 2009; Rostrup-Nielsen, 2006; Zhang et al., 2021b).

Following the shift reactions, hydrogen becomes the dominant component of the gas mixture, while carbon dioxide represents the primary carbon-containing product (Busca et al., 2024; Vogt et al., 2019; Zhang et al., 2021b).

The effective conversion of carbon monoxide in the shift section results in a hydrogen-rich gas stream with low impurity levels. This composition is particularly favorable for downstream purification using pressure swing adsorption. The concentration of carbon dioxide in a separable stream supports efficient CO_2 capture and is consistent with the objectives of blue hydrogen production (Bui et al., 2018; Kalman et al., 2022; Shabbani et al., 2024).

The mass balance results are in good agreement with reported data for commercial SMR plants, indicating that the modeled process realistically represents industrial hydrogen production behavior (Li et al., 2022; Rostrup-Nielsen, 2006; Zhang et al., 2021a).

Hydrogen Purity and Recovery

Hydrogen purification via pressure swing adsorption yields a final hydrogen product with purity

exceeding 97%, meeting the requirements of most industrial hydrogen applications. The prior removal of carbon dioxide reduces adsorbent loading and improves PSA performance, contributing to stable hydrogen purity and efficient separation (Kalman et al., 2022; Shabbani et al., 2024). The trade-off between hydrogen purity and PSA recovery is shown in Figure 7.

Figure 7
Relationship between hydrogen purity and PSA hydrogen recovery, illustrating the recovery–purity trade-off

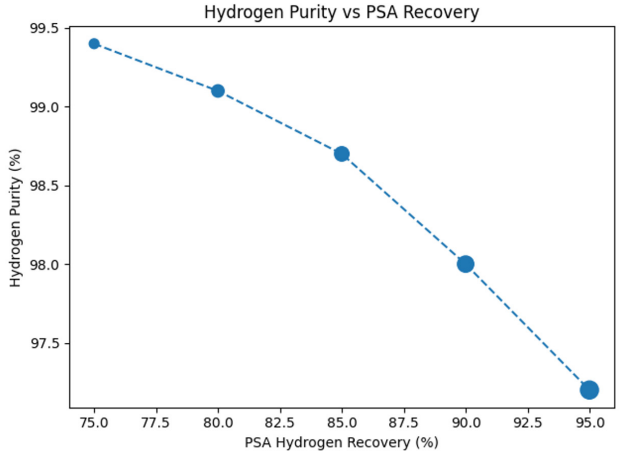


Figure 7 demonstrates the trade-off between hydrogen purity and PSA recovery. As recovery increases, a gradual decrease in product purity is observed due to stronger constraints on adsorption and regeneration performance. Nevertheless, the modeled operating window maintains hydrogen purity above 97%, which is consistent with industrial requirements for SMR-based hydrogen supply.

Hydrogen recovery losses associated with PSA operation remain within typical industrial ranges and are primarily linked to purge streams required for bed regeneration. Despite these losses, overall hydrogen recovery remains high, confirming effective utilization of the hydrogen produced in the reforming and shift sections (Kalman et al., 2022; Shabbani et al., 2024).

The achieved hydrogen purity and recovery are consistent with values reported in the literature for large-scale SMR-based hydrogen plants (Li et al., 2022; Shabbani et al., 2024; Zhang et al., 2021a).

Energy Demand and Thermal Integration

The energy analysis highlights the reforming section as the dominant contributor to overall process energy demand due to the strongly endothermic nature of steam methane reforming. Sustaining high reformer temperatures requires significant heat input, emphasizing the importance of efficient furnace design and fuel management in SMR systems (Rochelle, 2009; Rostrup-Nielsen, 2006). The distribution of energy demand among the main process units of the SMR-based hydrogen production system is shown in Figure 8.

Figure 8
Distribution of energy demand among the main process units of the SMR-based hydrogen production system

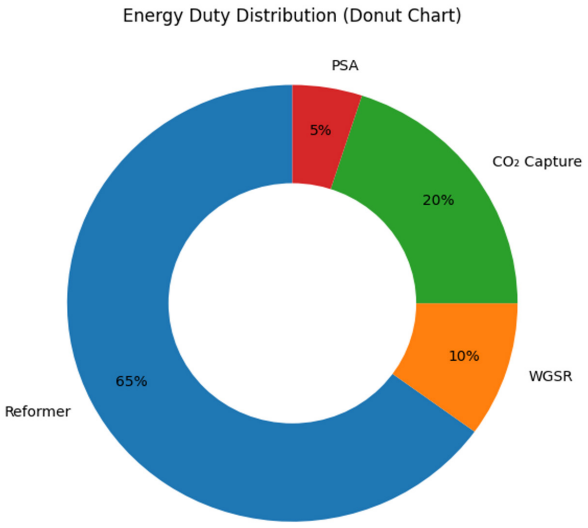


Figure 8 summarizes how the overall energy demand is distributed across the major process sections. The reformer dominates the energy balance due to the strongly endothermic character of steam methane reforming, while CO_2 capture represents the second-largest contribution associated with separation and regeneration duties. The WGSR and PSA sections require comparatively lower energy input.

In contrast, the water–gas shift reaction is mildly exothermic and contributes limited heat downstream of the reformer. Although this heat does not offset the reformer energy demand, it presents opportunities for recovery through steam generation or feed preheating. Such thermal integration strategies are critical for improving overall energy efficiency and reducing operating costs (Busca et al., 2024; Vogt et al., 2019; Wang et al., 2020; Zhang et al., 2021b). The incremental increase in energy demand associated with higher levels of CO_2 capture is shown in Figure 9.

Figure 9
Incremental increase in energy demand associated with higher CO_2 capture efficiency

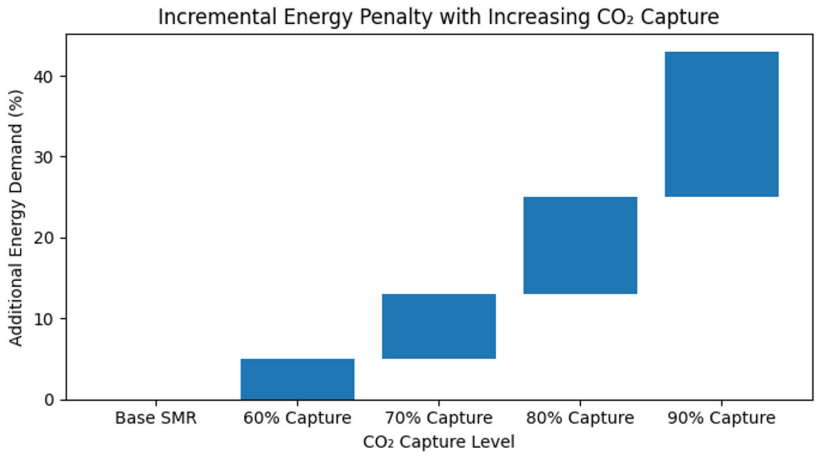


Figure 9 illustrates the incremental increase in energy demand associated with higher levels of CO_2 capture. As capture efficiency increases, additional energy requirements accumulate due to solvent regeneration and compression duties. While higher capture levels significantly reduce direct emissions, the results highlight a clear trade-off between emission reduction and energy consumption, which must be considered during process optimization.

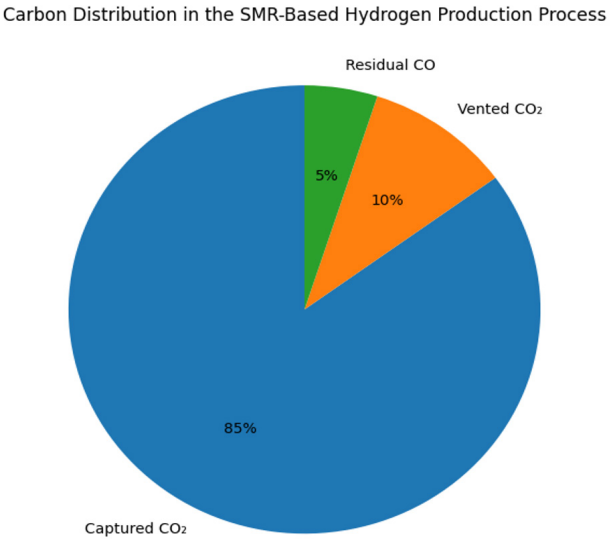
Additional energy requirements arise from carbon dioxide capture and hydrogen purification. In particular, solvent regeneration in the CO_2 absorption unit represents a notable energy penalty. This trade-off between energy consumption and emission reduction is characteristic of blue hydrogen systems and must be carefully evaluated in process design (Bui et al., 2018; Howarth & Jacobson, 2021; Quarton et al., 2020).

Effect of CO_2 Capture and Blue Hydrogen Implications

The integration of CO_2 capture significantly alters the carbon balance of the hydrogen production process. By removing the majority of carbon dioxide formed during reforming and shift reactions, the modeled system achieves a substantial reduction in direct CO_2 emissions compared with conventional SMR (Howarth & Jacobson, 2021; Luberti et al., 2022; Shahid & Kim, 2023). Distribution of carbon-containing species in the SMR-based hydrogen production process is shown in Figure 10.

Figure 10 presents the distribution of carbon-containing species within the modeled hydrogen production process. The majority of carbon is captured as carbon dioxide, while only a small fraction is released with the vent gas or remains as residual carbon monoxide. This distribution demonstrates the effectiveness of the integrated CO_2 capture system in reducing direct emissions and supports the classification of the process as a blue hydrogen production pathway.

Figure 10
Distribution of carbon-containing species in the SMR-based hydrogen production process



While CO_2 capture increases overall energy demand, the results indicate that hydrogen yield and product quality are not adversely affected. This finding supports the feasibility of integrating CO_2 capture into SMR-based hydrogen plants without

compromising core process performance (Bui et al., 2018; Quarton et al., 2020).

In regions with abundant natural gas resources and established industrial infrastructure, such as Kazakhstan, this configuration offers a realistic pathway for producing low-emission hydrogen. The results reinforce the role of SMR with CO_2 capture as a transitional blue hydrogen technology that can bridge the gap between conventional grey hydrogen and future large-scale deployment of renewable hydrogen (Hydrogen Council, 2021; IEAGHG, 2021; IEA, 2023, 2024; DOE, 2020, 2023). The comparison of specific CO_2 emissions for conventional SMR and SMR integrated with carbon dioxide capture is shown in Figure 11.

Figure 11
Comparison of specific CO_2 emissions for conventional SMR and SMR integrated with carbon dioxide capture

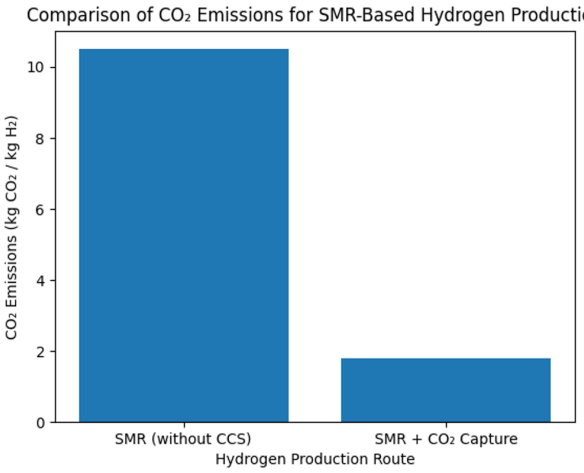


Figure 11 compares the specific CO_2 emissions associated with conventional SMR-based hydrogen production and SMR integrated with carbon dioxide capture. The incorporation of CO_2 capture results in a substantial reduction in direct emissions, decreasing the carbon intensity of hydrogen production by more than an order of magnitude. This comparison highlights the effectiveness of carbon capture integration in transforming conventional SMR into a low-emission blue hydrogen pathway.

Overall, the simulation results demonstrate that the integration of steam methane reforming, water–gas shift conversion, and carbon dioxide capture enables efficient hydrogen production with significantly reduced carbon emissions. The analyzed process configuration achieves high hydrogen yield and purity while maintaining industrially realistic operating conditions. Although the inclusion of CO_2 capture introduces additional energy demand, the substantial reduction in emissions confirms the technical viability of SMR-based blue hydrogen as a transitional solution for large-scale hydrogen production. The key performance indicators obtained from the process simulation are summarized in Table 2.

Table 2
Key performance indicators of the modeled SMR-based hydrogen production system

Performance indicator	Value
Methane conversion	>90%
Hydrogen yield	Near thermodynamic limit
Hydrogen purity	>97%
CO_2 capture rate	~90%
Specific CO_2 emissions (with capture)	~1.8 kg CO_2 / kg H_2
Dominant energy consumer	Reformer

Feasibility Analysis

Feedstock and Infrastructure Availability

The feasibility of hydrogen production via steam methane reforming with integrated CO_2 capture is strongly influenced by the availability of natural gas and supporting infrastructure. Regions with established gas supply networks, processing facilities, and industrial consumers offer clear advantages for SMR-based hydrogen deployment. Kazakhstan possesses significant natural gas reserves and a well-developed gas transportation system, which provides a reliable and cost-effective feedstock supply for hydrogen production (Hydrogen Council, 2021; IEA, 2023, 2024; DOE, 2020, 2023).

In particular, the western regions of Kazakhstan host major oil and gas operations, refineries, and petrochemical facilities. Existing infrastructure reduces the need for extensive new pipeline construction and enables direct integration of hydrogen production units into current industrial complexes. Such integration is especially beneficial for SMR-based systems, which rely on continuous gas supply and stable operating conditions (Abdalla et al., 2018; Dincer & Acar, 2015; Staffell et al., 2019; DOE, 2020, 2023).

Industrial Integration Potential

One of the key advantages of SMR-based hydrogen production lies in its compatibility with existing

industrial hydrogen consumers. In Kazakhstan, hydrogen is already used internally in petroleum refining for hydrotreating and hydrocracking processes. Locating a dedicated hydrogen production unit near refineries or petrochemical plants allows direct utilization of hydrogen without the need for long-distance transport or storage infrastructure (Staffell et al., 2019; DOE, 2020, 2023).

The Atyrau region represents a particularly favorable location due to the presence of large refineries, petrochemical facilities, and associated utilities. Co-location with existing plants enables the sharing of steam systems, cooling water, power supply, and maintenance services, thereby reducing capital and operating expenditures. In addition, the availability of skilled technical personnel further enhances project feasibility (Hydrogen Council, 2021; IEA, 2023, 2024; DOE, 2020, 2023).

Carbon Capture and Storage Considerations

The feasibility of blue hydrogen production critically depends on the ability to manage captured carbon dioxide. In the modeled process, CO_2 is produced in a concentrated stream downstream of the water–gas shift reaction, which is well suited for capture using chemical absorption. This configuration minimizes separation complexity and improves capture efficiency (Bui et al., 2018; Shahid & Kim, 2023).

For long-term emission reduction, captured CO_2 must be either utilized or stored. Kazakhstan has geological formations with potential for CO_2 storage, including depleted oil and gas reservoirs. Integration of CO_2 capture with existing oil and gas operations could enable carbon storage or enhanced oil recovery applications. However, further site-specific geological assessment would be required to confirm storage capacity, integrity, and long-term safety (Bui et al., 2018; IEAGHG, 2021).

Economic and Transitional Perspective

From an economic standpoint, SMR with CO_2 capture represents a transitional solution between conventional grey hydrogen and renewable green hydrogen. While green hydrogen offers the lowest emissions, its current production costs and dependence on large-scale renewable electricity limit near-term deployment in many regions. In contrast, blue hydrogen leverages existing SMR technology and infrastructure, allowing faster implementation at lower capital risk (Howarth & Jacobson, 2021; Luberti et al., 2022; Nazir et al., 2020; Quarton et al., 2020). A comparison between conventional SMR and SMR integrated with CO_2 capture is summarized in Table 3.

Table 3
Comparison of conventional SMR and SMR-based hydrogen production with CO_2 capture

Parameter	Conventional SMR (Grey H_2)	SMR with CO_2 capture (Blue H_2)
Hydrogen purity	>97%	>97%
Methane conversion	High	High
CO_2 emissions	~10–12 kg CO_2 / kg H_2	~1.5–2 kg CO_2 / kg H_2
Energy demand	Lower	Higher
CO_2 capture requirement	Not applied	Required
Technology maturity	Commercial	Commercial
Emission profile	High	Significantly reduced

The additional energy demand associated with CO_2 capture increases operating costs compared with conventional SMR. However, these costs may be partially offset by regulatory incentives, carbon pricing mechanisms, or demand for low-emission hydrogen in international markets. In this context, blue hydrogen can serve as an intermediate step that supports gradual decarbonization while maintaining industrial competitiveness (Hydrogen Council, 2021; IEAGHG, 2021; IEA, 2023, 2024; Shahid & Kim, 2023; DOE, 2020, 2023).

Limitations and Future Outlook

Although the feasibility analysis indicates strong potential for SMR-based blue hydrogen deployment, several limitations must be acknowledged. The economic viability of CO_2 capture depends on energy prices, solvent performance, and access to storage or utilization pathways. Furthermore, methane emissions associated with upstream natural gas supply can influence the overall climate impact of blue hydrogen (Bui et al., 2018; Howarth & Jacobson, 2021; Luberti et al., 2022; Shahid & Kim, 2023).

In the long term, the role of SMR-based hydrogen is expected to evolve as renewable hydrogen technologies mature and become more cost competitive. Nevertheless, in the near to medium term, SMR with CO_2 capture provides a realistic and scalable option for reducing emissions from hydrogen production in regions with abundant natural gas resources (Belmehdi et al., 2025; Hydrogen Council, 2021; IEA, 2023, 2024; Nazir et al., 2020; Quarton et al., 2020; DOE, 2020, 2023).

Conclusion

In this study, hydrogen production via steam methane reforming integrated with the water–gas shift reaction and carbon dioxide capture was analyzed using a detailed process simulation approach. An industrially relevant SMR–WGSR configuration was modeled in Aspen HYSYS to evaluate hydrogen yield, product purity, energy demand, and the impact of CO_2 capture under steady-state operating conditions. The results demonstrate that the selected process configuration enables high methane conversion and hydrogen yields approaching thermodynamic limits, while delivering hydrogen at purity levels suitable for industrial applications (AspenTech, 2021; Li et al., 2022; Moioli et al., 2024; Zhang et al., 2021a).

The integration of the water–gas shift reaction was shown to play a critical role in maximizing hydrogen production by converting carbon monoxide into additional hydrogen and carbon dioxide. Downstream purification using pressure swing adsorption achieved hydrogen purity exceeding 97%, confirming the suitability of the modeled system for large-scale hydrogen supply. Although steam methane reforming remains energy intensive due to the strongly endothermic nature of reforming reactions, opportunities for heat recovery and thermal integration were identified as essential elements for improving overall process efficiency (Busca et al., 2024; Kalman et al., 2022; Rochelle, 2009; Rostrup-Nielsen, 2006; Shabbani et al., 2024; Vogt et al., 2019; Zhang et al., 2021b).

The inclusion of carbon dioxide capture substantially reduces direct CO_2 emissions compared with conventional SMR-based hydrogen production. While CO_2 capture introduces additional energy requirements, particularly for solvent regeneration, the overall hydrogen yield and product quality remain largely unaffected. This trade-off highlights the potential of SMR with carbon capture as a viable blue hydrogen pathway, capable of balancing emission reduction with industrial performance (Bui et al., 2018; Howarth & Jacobson, 2021; Luberti et al., 2022; Shahid & Kim, 2023; Quarton et al., 2020).

From a regional perspective, the feasibility analysis indicates that countries with abundant natural gas resources and established industrial infrastructure, such as Kazakhstan, are well positioned to deploy SMR-based blue hydrogen systems. The Atyrau region, in particular, offers favorable conditions for integration with existing refineries and petrochemical facilities, enabling efficient utilization of hydrogen and supporting infrastructure sharing. In the near to medium term, SMR with CO_2 capture represents a realistic transitional solution that can support decarbonization goals while maintaining reliable hydrogen supply for industrial consumers (Hydrogen Council, 2021; IEAGHG, 2021; IEA, 2023, 2024; DOE, 2020, 2023).

Overall, the findings of this study support the role of SMR-based blue hydrogen as an important component of the evolving hydrogen economy. While long-term decarbonization will increasingly rely on renewable hydrogen pathways, integrated SMR–WGSR systems with carbon capture can provide a scalable and technologically mature solution for reducing emissions from hydrogen production during the transition period (Howarth & Jacobson, 2021; Luberti et al., 2022; Nazir et al., 2020; Quarton et al., 2020).

Author contributions

Author Conceptualization, methodology, and writing – original draft preparation: D.S. and Y.K.; investigation, data curation, and formal analysis: B.S., T.T., and T.A.; visualization and validation: A.K.; supervision and writing-review and editing: Y.K. and T.A.; project assignment, scientific guidance, and final verification: A.I.

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Conflicts of interest

The authors declare no conflict of interest.

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