

# Synthesis and Optimization of Integrated Hydrogen Production and Supply Network for Multi-Plant Scenario

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This study presents a method for the synthesis and optimization of an integrated onsite hydrogen production and associated supply chain network for petroleum refinery plants that utilize grey, blue, and green hydrogen to meet operational demand. The primary objectives are to minimize carbon emissions and total annual cost (TAC). The study formulates the problem as a Mixed Integer Nonlinear Programming model using General Algebraic Modelling System, aiming to balance economic and environmental objectives. The goal is to identify the optimal production mix and hydrogen supply chain that achieves the lowest possible carbon footprint while maintaining cost efficiency. In the cost-minimization scenario, the optimal production mix consisted of 80 % steam methane reforming (SMR) and 20 % SMR with carbon capture (SMRCCS), resulting in the lowest TAC of \$  $0.88 \times 10^6$ . In contrast, the emission-minimization scenario favoured a mix of 80 % electrolysis and 20 % SMRCCS, achieving the lowest CO<sub>2</sub> emissions at 0.0123 t/y. A balanced, multi-objective optimization with equal weighting between cost and emissions reduced emissions by 37.34 % compared to the cost-optimal case, highlighting the potential for substantial environmental benefits with moderate cost trade-offs. This framework supports refineries in transitioning to sustainable hydrogen production.

## 1. Introduction

The global energy sector is transforming towards sustainability, driven by the urgent need to reduce carbon emissions and mitigate climate change. Hydrogen is an important chemical resource extensively used in the petrochemical industry. Refinery hydrogen management systems are marked by substantial hydrogen requirements, which vary in terms of purity level and pressure for oil refining (Zhou et al., 2024). The increased supply of heavy crude oil and increasingly stringent environmental regulations have resulted in more use of hydrogen in refineries to produce lighter fuels and cleaner commodities (Chang, 2022). Hydrogen is regarded as an upgrading agent for crude oil products and petroleum distillates in terms of hydrocracking and hydrotreating processes. The refinery hydrogen management system is comprised of hydrogen-producing streams (hydrogen sources) that supply hydrogen to hydrogen-consuming streams (hydrogen sinks). Internal hydrogen sources within the refinery cannot satisfy the overall hydrogen demand, hence the need for fresh sources of hydrogen. Given the significance of hydrogen in the refinery sector, onsite production is a more practical approach. Optimizing the integration of internal hydrogen sources and sinks remains necessary to minimize the need for fresh hydrogen and lower operational expenses. To overcome economic and environmental challenges, optimizing the synthesis of refinery hydrogen management systems has been a key research focus for an extended period.

Several techniques and approaches have been developed and investigated, and the two renowned approaches to designing hydrogen network synthesis and optimization are Pinch Analysis (PA) and mathematical programming (Ibrahim and Al-Mohannadi, 2023). PA provided thermodynamic insights for minimizing fresh hydrogen consumption, though they often overlooked pressure constraints and complex operational factors. Mathematical programming methods have also been employed to develop superstructure-based optimization methods to solve optimization problems addressing the limitations of PA. Mathematical modelling allows a comprehensive approach as it considers possible alternatives to synthesize any process or system (Loh et al., 2024). Researchers such as Ibrahim and Al-Mohannadi (2023) developed a mixed integer non-linear

programming (MINLP) model to optimize low-carbon hydrogen supply chain networks (HSCNs) in industrial clusters, aiming to minimize the levelized cost of hydrogen while meeting CO<sub>2</sub> emission reduction targets. The economic viability of hydrogen supply chains is a central focus of research, as highlighted by Ibrahim and Al-Mohannadi (2023), who provide detailed economic and technical data for hydrogen production, conditioning, storage, and transportation. Their work emphasizes the cost structures of various production methods, including SMR, coal gasification, biomass gasification, and water electrolysis. Hydrogen production, traditionally reliant on fossil fuel-based processes like SMR, generates substantial carbon dioxide (CO<sub>2</sub>), contributing to the environmental footprint of refineries. Emerging technologies, such as hydrogen production via water electrolysis powered by renewable energy and SMR with carbon capture and storage (CCS), offer pathways to decarbonize hydrogen supply chains.

Hydrogen production processes are categorized based on the feedstock used, the technology applied, and the associated CO<sub>2</sub> emissions (Ahn et al., 2023). Hydrogen produced from fossil fuels is called grey hydrogen, due to the greenhouse gas (GHG) emissions generated during its production. By incorporating CO<sub>2</sub> capture and sequestration into fossil-based production, the resulting hydrogen is known as blue hydrogen. The other route that is receiving significant interest, which has the potential to achieve very low to zero emissions, is water electrolysis using clean or renewable electricity, referred to as green hydrogen. The integration of sustainable hydrogen production into refinery operations has gained significant attention in recent years, driven by the need to align industrial processes with global decarbonization goals. The study by Zhou et al. (2024) investigates the integration of renewable energy, specifically wind power, into refinery hydrogen management systems, focusing on energy storage and direct utilization to address the intermittency of renewable resources. The findings demonstrate the economic viability of using wind power for hydrogen production to reduce costs and enhance sustainability. Lal and You (2022) did a comprehensive comparative life cycle analysis of brown (referred to as grey hydrogen in this study) and blue hydrogen production pathways, focusing on SMR with and without CCS. Their work highlights the optimization of operating conditions such as temperature, pressure, and steam-to-methane ratio to minimize global warming potential (GWP) and operating costs. Under optimal conditions, the blue hydrogen pathway achieved a 33 % lower GWP compared to brown hydrogen, while the brown hydrogen pathway had up to 69 % lower operating costs. These findings emphasize the trade-offs between cost and environmental impact in hydrogen production and highlight the potential of process optimization and technological integration to advance a sustainable hydrogen economy.

This paper addresses the synthesis and optimization of an integrated onsite hydrogen production and supply chain for petroleum refineries, merging grey, blue, and green hydrogen production methods. The paper aims to balance economic and environmental objectives, minimizing both carbon emissions and production costs. The paper evaluates key hydrogen production technologies, including SMR with and without CCS and water electrolysis, to determine the optimal production mix energy supply chain configuration that achieves cost efficiency and reduced carbon emissions. Grey and blue hydrogen typically require post-production purification to meet the >99.9 % purity standards demanded by refinery processes, due to the presence of impurities such as CO<sub>2</sub> and CH<sub>4</sub> from fossil-based production routes (Ibrahim and Al-Mohannadi, 2023). In contrast, green hydrogen produced via electrolysis generally achieves ultra-high purity (>99.999 %) with negligible contaminants, eliminating the need for further purification before refinery use. The design of sustainable hydrogen supply chains for industrial applications, such as refineries, requires a holistic approach that integrates production and distribution. Isafiade and Short (2022) propose a novel method for integrating renewable energy feedstock supply chains (e.g., corn stover, glycerine, wood) with combined heat and power (CHP) generation hubs and heat exchanger networks (HENS), optimizing TAC and environmental impact through a weighted sum approach. The integration of renewable feedstocks with CHP and HENS parallels the challenges of optimizing hydrogen purification for multiple refineries. Isafiade and Short (2022) emphasize the economic and environmental advantages of a centralized energy hub, which reduces capital and operating costs by leveraging economies of scale and minimizes emissions through strategic feedstock selection. This work contributes to the goal of sustainable energy transitions by providing a framework for refinery operators to integrate low-emission hydrogen production strategies effectively.

## 2. Problem statement

The problem formulation can be stated as follows. Consider a set of onsite hydrogen production technologies, PT, to supply a set of co-located refineries R, each with specific seasonal hydrogen demands characterized by flow rates. The objective is to determine the optimal production mix of grey hydrogen (via steam methane reforming without CCS), blue hydrogen (via steam methane reforming with CCS), and green hydrogen (via water electrolysis) to meet demand while minimizing TAC and carbon emissions. The proposed superstructure for the hydrogen production model and supply chain is shown in Figure 1. The superstructure is comprised of three layers, the first layer includes energy feedstock supply, while the second layer is comprised of the production

technologies with the option to include a purification hub utilising pressure swing adsorption. The third layer consists of product distribution, that is, CO<sub>2</sub> purge for SMR, CO<sub>2</sub> capture for SMRCCS, O<sub>2</sub> purge for electrolysis, and H<sub>2</sub> transfer to refineries. Key decisions involve selecting the production mix, optimizing supply routing to meet hydrogen demand, and integrating carbon mitigation technologies, such as CCS for blue hydrogen, to balance economic and environmental objectives.

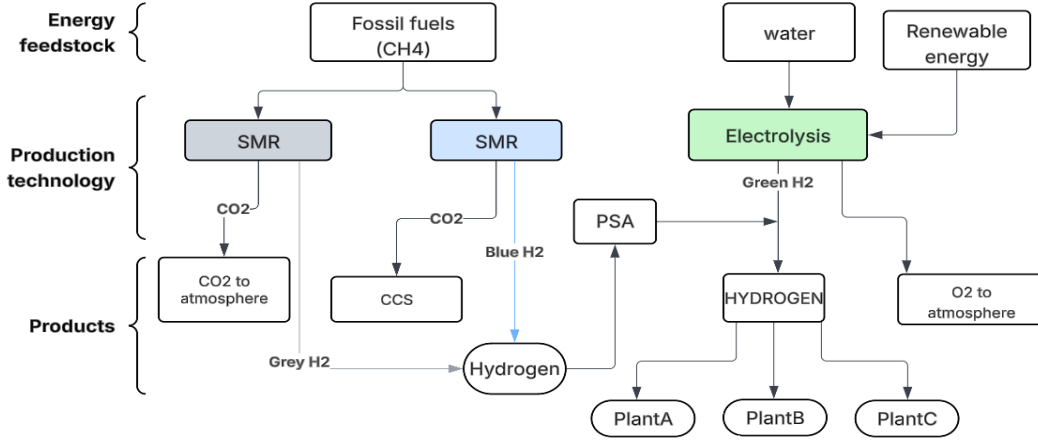


Figure 1: Hydrogen production model superstructure

### 3. Methodology

The integrated supply chain and hydrogen production model was developed to optimize hydrogen production to meet the demand for co-located refineries (Plant A, Plant B, Plant C), considering economic and environmental objectives. Hydrogen production is modeled for three technologies: SMR, SMRCCS, and water electrolysis, producing grey, blue, and green hydrogen, respectively. Each technology is characterised by production capacity, power demand, carbon emissions, investment, and operating costs. The same nominal production capacity was assigned to grey, blue, and green hydrogen production technologies in the model to maintain consistency and comparability across the different production pathways. This assumption is justified by the need to standardize the spatial and infrastructural requirements at refinery sites. Employing uniform capacity values allows a more controlled assessment of cost and emissions performance, ensuring that variations in results are not influenced by differences in scale but by technological characteristics. Hydrogen demand is specified for each refinery and season, with total production set to at least meet or exceed demand. The key input parameters were obtained from relevant literature and were selected based on their consistency with recent studies in the field of hydrogen supply chains and carbon mitigation systems to ensure that the model reflects realistic and credible assumptions. In cases where literature presented a range of values, representative averages were adopted to preserve modeling consistency.

#### 3.1 Optimization objective and case study

The model was tested on a case study involving three refinery plants with varying hydrogen demands across three seasons of the year, as shown in Table 1. Hydrogen demand in refineries tends to vary with the seasons, influenced by changes in fuel specifications, weather patterns, and operational needs (He et al., 2025). The model minimizes a multi-objective function combining TAC ( $10^6$  \$/y) and carbon emissions (t/y), as shown in Eq(1), where  $w$  is the weighting factor ranging between 0 and 1,  $C_{obj}$  ( $10^6$  \$/y) is the cost objective and  $E_{obj}$  (t/y) is the emissions objective.

$$\text{Objective function} = \text{minimize} (w \cdot C_{obj} + (1 - w) \cdot E_{obj}) \quad (1)$$

$$C_{obj} = TAC_{SMR} \cdot y + TAC_{SMRCCS} \cdot z + TAC_{Electrolysis} \cdot x \quad (2)$$

$$E_{obj} = \sum_{s \in S} FC_{SMR,s} \cdot y + \sum_{s \in S} FC_{SMRCCS,s} \cdot z + \sum_{s \in S} FC_{Electrolysis,s} \cdot x \quad (3)$$

$$FH_{SMR,s} \leq Cap_{SMR} \cdot y \quad (4)$$

$$FH_{SMRCCS,s} \leq Cap_{SMRCCS} \cdot z \quad (5)$$

$$FH_{Electrolysis,s} \leq Cap_{Electrolysis} \cdot x \quad (6)$$

$$Power\ demand_{SMR,s} = PPower_{SMR} \cdot FH_{SMR,s} \quad (7)$$

$$Power\ demand_{SMRCCS,s} = PPower_{SMRCCS} \cdot FH_{SMRCCS,s} \quad (8)$$

$$Power\ demand_{Electrolysis,s} = PPower_{SMR} \cdot FH_{SMR,s} \quad (9)$$

$$Operating\ cost_{SMR,s} = OPC_{SMR} \cdot FH_{SMR,s} \cdot PPower_{SMR} + PC_{SMR,s} \quad (10)$$

Eq(2) illustrates the calculation of  $C_{obj}$ , which is the summation of the TAC for all the individual technologies multiplied by their respective binary variables,  $y$ ,  $z$ , and  $x$ , indicating use of SMR, SMRCCS, and Electrolysis, respectively. The emission objective  $E_{obj}$  shown in Eq(3) is the total of all emissions from operating the three production technologies across the year, where  $FC$  (t/y) is the flow rate of  $CO_2$  emitted per season  $s$  for each technology. The value of  $FC$  in season  $s$  for SMR ( $FC_{SMR,s}$ ) and SMRCCS ( $FC_{SMRCCS,s}$ ) is derived from the reaction of methane to form  $H_2$  and  $CO_2$  during steam methane reforming. While electrolysis does not emit  $CO_2$  during operation, its true environmental performance hinges on the carbon intensity of the electricity source. In this study, electrolysis is assumed to operate using grid electricity; hence, the technology's arbitrary but conservative emission value was assigned to reflect its likely environmental impact, and this is the source of the  $FC$  value for electrolysis. Eq(4) shows the production capacity constraint for SMR, where  $FH_{SMR}$  (t/y) is the flow rate of hydrogen produced, and  $Cap_{SMR}$  (tH<sub>2</sub>/h) is the parameter for SMR production capacity. This equation is applied to all three technologies with their respective binary variables as shown in Eq(4), Eq(5) and Eq(6) for all three technologies. The use of binary variables in Eq(2) to Eq(6) allows the model to select the optimal production technology. Eq(7) to Eq(9) calculate the power demand for each of the technologies.  $PPower$  (kWh/tH<sub>2</sub>) in these equations is the power demand parameter for each technology, which represents the amount of energy required per ton of hydrogen produced, and it significantly influences the overall TAC. Eq(10) calculates the overall operating cost (\$/kW), which includes the cost of power,  $PC$  (\$/kW) for SMR. The equivalent of Eq(10) are also implemented for the other two technologies. The differences in energy demand arise from the underlying processes: SMR and SMRCCS use thermal and catalytic reactions with natural gas, which are relatively energy-efficient, whereas electrolysis splits water molecules using electricity, a process that is inherently more energy-intensive. Table 2 shows some input parameters used for the different technologies in solving the model. In this table, capacity determines the scale of output, investment cost (\$/kW), and operating cost (OPC (\$/kW)) parameters, directly impacting the initial capital required to build the facility and the ongoing expenses needed to keep it running. The rest of the data used for the case study can be found in the supplementary file Mufanabadza et al. (2025). The integrated hydrogen supply chain optimization model was implemented in GAMS (GAMS Development Corporation, 2015) and solved using the DICOPT solver. The model has 40 blocks of equations, 1,232 single equations, 17 blocks of variables, 97 single variables, and 3 discrete variables.

Table 1: Hydrogen demand

Plant	Hydrogen demand (tH <sub>2</sub> )		
	Season 1	Season 2	Season 3
Plant A	0.126	0.125	0.124
Plant B	0.115	0.117	0.116
Plant C	0.130	0.128	0.127

Table 2: Model input parameters (Ahn et al., 2023)

Parameters	SMR	SMRCCS	Electrolysis
Capacity (tH <sub>2</sub> /h)	0.3	0.3	0.3
Investment cost (\$/kW)	1,120	1,991	1,500
OPC (\$/kW)	52.64	59.63	49.28
PPower (kWh/tH <sub>2</sub> )	8,240	9,000	52,000

#### 4. Results

Three optimization scenarios were analyzed to evaluate trade-offs between economic and environmental objectives, and the results are shown in Table 3. Table 4 shows the flow rate of H<sub>2</sub> being sent to each plant from each of the hydrogen production technologies. First, a cost-minimization scenario was conducted to identify the most economically efficient production technology. The model selected a combination of SMR, producing 80 % of the total hydrogen supply, and SMRCCS with a TAC value of \$ 0.88 x10<sup>6</sup>. SMR technology has the least TAC value, but since its capacity cannot satisfy the hydrogen demand, the balance is produced by the next least expensive technology, which is blue hydrogen. Despite its relatively high emissions, SMR remains the least-cost technology due to mature infrastructure, established supply chains, and low natural gas prices. This scenario stresses the persistent role of grey and blue hydrogen in the near term, particularly when capital and operational costs dominate the decision-making criteria. Secondly, an emission-minimization scenario was examined to identify the technology with the least emissions, regardless of cost, shifting the focus towards decarbonization. Electrolysis and SMRCCS were selected as the optimal production mix with an 80:20 ratio towards demand satisfaction. The selection of these technologies for the emissions objective aligns with the global trends toward blue and green hydrogen to decarbonize industrial processes. The best value for the emissions objective was 0.0123 t/y. This affirms the feasibility of low-emission hydrogen pathways and their role in industrial decarbonization targets.

Table 3: Results obtained for the three scenarios

Scenarios	H <sub>2</sub> flowrate (t/y)			TAC (x10 <sup>6</sup> \$)	CO <sub>2</sub> emissions (t/y)
	SMR	SMRCCS	Electrolysis		
1. Cost objective	0.900	0.213	0.000	0.882	0.233
2. Emissions objective	0.000	0.213	0.900	10.060	0.014
3. Multi-objective	0.213	0.900	0.000	1.023	0.087

Table 4: Hydrogen flow rate to each plant for the three scenarios

Scenarios	Plant	H <sub>2</sub> flowrate t/y		
		SMR	SMRCCS	Electrolysis
1	A	0.305	0.072	0.000
	B	0.283	0.067	0.000
	C	0.313	0.074	0.000
2	A	0.000	0.072	0.305
	B	0.000	0.067	0.283
	C	0.000	0.074	0.313
3	A	0.072	0.305	0.000
	B	0.067	0.283	0.000
	C	0.074	0.313	0.000

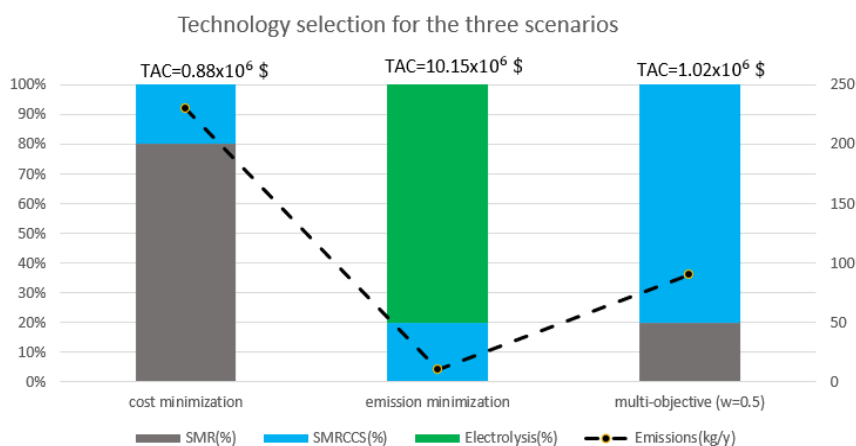


Figure 2: Technology selection for the three scenarios.

Finally, a series of multi-objective optimization runs were performed using the weighted sum approach, simulating different stakeholder preferences. The equal weighting ( $w = 0.5$ ) of the two objectives achieved a 37.34 % reduction in CO<sub>2</sub> emissions compared to the first scenario relying on grey and blue hydrogen. The balanced solution employs a hybrid production strategy where SMR is deprioritized due to its high emissions. Figure 2 shows a summary of the results obtained. Blue hydrogen was picked in all scenarios due to its favorable balance between costs and emissions. This consistent selection underscores its strategic value as a transitional enabler between fossil-based hydrogen production methods and future green hydrogen solutions. Minor increases in cost can result in substantially greater reductions in emissions, thereby presenting mutually beneficial outcomes within the context of well-structured policy frameworks. The production mix demonstrates the importance of context-specific decision-making, particularly under variable energy prices and carbon taxes.

## 5. Conclusions

This study formulated an MINLP model to optimize an integrated hydrogen production and supply network in refineries, striking a balance between cost and carbon emissions. The results show that green hydrogen has the least carbon emissions, highlighting its environmental superiority. However, grey hydrogen production remains the most cost-effective. Though CCS processes reduce direct CO<sub>2</sub> emissions, many researchers have argued that it is better to produce hydrogen in ways that do not produce CO<sub>2</sub> rather than investing in abatement technologies. However, the possibility of retrofitting carbon capture technology in existing SMR plants can help reduce the costs associated with the transition to cleaner hydrogen production. To further facilitate the widespread adoption of green hydrogen, implementing supportive policy instruments such as subsidies, tax incentives, or carbon pricing mechanisms could substantially improve its economic viability. For example, government support for renewable energy initiatives or the imposition of penalties on carbon-intensive hydrogen production may help close the gap, thereby enhancing the competitiveness of green hydrogen relative to grey and blue alternatives in industrial sectors such as refineries. Future work could look at different grid setups or renewable energy systems to better understand how electrolysis fits into a low-carbon hydrogen economy. As the hydrogen economy matures, the ability to adaptively balance cost, emissions, and demand across regions and seasons will be critical to achieving both short-term feasibility and long-term sustainability.

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