

Modelling and Optimization of Hydrogen Production in an Industrial Cluster Accounting for Economic Cost and Environmental Impact

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According to the Paris agreement and under emissions reduction protocols, the global energy sector is expected to abide by the established restrictions to target zero-carbon resources by 2050. Hydrogen has been known as one of the most plentiful elements in the universe, yet it solely appears as combined with other elements. Therefore, hydrogen production itself is an energy-intensive process and thus could generate significant amounts of CO₂. Nevertheless, green hydrogen (produced from renewable resources) rapidly gaining interest as a key material in the decarbonisation of the energy sector and one of the promising solutions to tackle the global warming challenge. This work presents a framework for hydrogen and CO₂ utilisation strategies in an industrial park while identifying optimum decisions related to the allocation of the feedstock through possible technologies to produce sustainable and low-cost hydrogen. A techno-economic optimization model based on a superstructure approach has been developed to identify the best possible hydrogen network configurations from a number of technologies, which is achieved by a combination of many possible hydrogen and CO₂ utilisation scenarios. A case study that resembles Qatar's industrial economy is set out to investigate the application of the proposed approach.

1. Introduction

The Intergovernmental Panel on Climate Change (IPCC) establishes an emissions reduction protocol to cap the global temperature rises at 1.5 °C by targeting zero-emissions resources goal by 2050 (IPCC, 2018). Currently, 80% of the global energy demand is driven by resources that contain carbon resulting in a continuous release of emissions into the atmosphere (IEA, 2019). These emissions generate from hard-to-abate sectors and applications; therefore, deep decarbonization of these sectors is hard to achieve in the near term. Hydrogen has been identified as a key material that can help abate emissions in the energy sector due to its high energy density and clean energy carrier nature. Even though hydrogen is the most abundant element in the universe, hydrogen is not readily available as an energy source. Hydrogen is usually available as water, hydrocarbons (e.g., methane), and other organic components. The separation of hydrogen requires energy that could produce emissions. Thus, there is a need to be extracted efficiently from these compounds. Today 48% of the approximately 120 million tons of hydrogen worldwide is from natural gas (IRENA, 2019), accompanied by a significant amount of CO₂ emission as a result of converting the natural gas catalytically to hydrogen (David Joffe, 2018). Another option to produce hydrogen is water electrolysis. The downside of this technology is that it requires a significant amount of electricity (IRENA, 2018). Renewable energy sources can be used to supply power that can offset emissions, but continuous production at a large scale is still an issue.

Analysis through process systems engineering (PSE) tools could be used to analyze hydrogen production systems. In addition, Process Integration (PI) approaches, as one of the major practical techniques of PSE, could be utilized in the minimization of energy required, raw materials demand, and waste generation. In the context of hydrogen, many works in PSE have investigated hydrogen management through Hydrogen Network Integration (HNI) to support increasing hydrogen demand at an acceptable price. HNI approaches fall into categories, graphical and mathematical programming. The most common graphical approach in hydrogen management is Hydrogen Pinch Analysis (HPA), first developed by Alves and Towler (2002). The approach is

analogous with water and energy pinch methods, and since its inception, numerous enhancements have been developed. Zhao et al(2007) introduced a new graphical method to handle the problems with multiple impurities. Ding et al. (2011) proposed the average pressure profile of the sources and the sinks to overcome the pressure limitation of the original method. Foo and Manan (2006) developed the Gas Cascade Analysis (GSA) tool to develop a quick and accurate method to identify the fresh hydrogen flow rate target. On the other hand, many mathematical programming methods have emerged to cope with the limitations of the graphical technique. A hydrogen network was first optimized by Hallale and Liu(2001). Liu and Zhang(2004) extended the superstructure to select the appropriate purifier (e.g., membranes, pressure swing adsorption, and hybrid system) to achieve the optimum flowsheet configuration. Detailed descriptions as well as state-of-art by highlighting the earliest contribution for the hydrogen process integration are reported by Elsherif et al (2015), and Marques et al (2017).

Previous research has focused on investigating the economic aspect of the hydrogen network; however, few studies addressed simultaneous environmental and economic aspects of hydrogen management at a cluster level. One of the few studies that handled these two metrics simultaneously was done by Zhou et al(2013). They developed an optimal synthesis of sustainable hydrogen network; nevertheless, Zhou et al (2013) do not utilize or merge the CO₂ with Carbon Capture Utilisation and Storage (CCUS). Al-Mohannadi et al (2020) looked into natural gas and CCUS using a mathematical technique, yet it only focused on two materials. Ahmed et al (2020), introduced a Resource Integration optimization model based on a novel representation that allows exploring the exchange of materials and energy resources, including intermediates, emissions, and wastes. The interaction is enabled through pre-specified resource lines with known temperature, pressure, and purity connected to all plants and allows the exchange of any resource. Hence, this study is set out to investigate the hydrogen production and utilisation network while managing carbon dioxide through the resource integration technique.

2. Problem Statement

This work aims to develop a network for minimizing the total cost of hydrogen and the CO₂ emissions associated with hydrogen production. The hydrogen network described in this work is composed of several Hydrogen production and chemical production plants for CO₂ that utilize hydrogen and CO₂ as feedstock. Following Ahmed et al(2020) approach, each plant in the cluster is connected to a unique central infrastructure with pre-specified materials at a given condition (namely temperature, pressure, and purity) that are allowed to be exchanged within the cluster. The inputs and outputs of each plant or process can be obtained from the infrastructure. Each plant can emit a certain amount of CO₂, and the cluster's CO₂ emissions are comprised of all individual plant emissions, which are constrained to a total allowable footprint. A power grid with mixed energy options has been considered, including a conventional power grid that takes natural gas as raw material and renewable energy options. The cluster can also have several treatment facilities to treat input resources such as water or treat waste such as carbon capture units to concentrate carbon dioxide. For each plant, process, or treatment, the capital and operating costs are calculated. The profit is generated through the sale of hydrogen and chemical byproducts exported outside the cluster. Hence, the optimization problem stated in this study can decide:

- Hydrogen production plant options to be selected in the cluster,
- The capacity of the hydrogen production from production plants,
- Power grid mix required,
- Allocation of hydrogen utilisation proposed plants in the cluster (possible sinks),
- Allocation of CO₂ captured and treated to possible sinks or utilisation.

3. Model Formulation

This work adopted the resources integration method and corresponding optimization model from Ahmed et al (2020), and customized to analyse hydrogen production in an industrial clusters. The mixed integer linear program models the process through mass and energy balances utilizing linear input/output parameters to account for material and energy demands. The objective is to minimize the total cost of the network as follows:

$$\text{Min Cost} = \sum_p cc_p^{CAPEX} C_p + \sum_r IF_r \beta_r + \sum_p (ao_p^{variable} C_p + ao_p^{Fixed}) - \sum_r OR_r \beta_r \quad (1)$$

The revenue is obtained by selling the hydrogen as well as all the added-value products price of β_r and output flow OR_r for each resource r . The capital cost and is the summation of annualized capital costs of all individual plants in the cluster where C_p is the capacity of the process p and process cc_p^{CAPEX} is the process's p annualized capital cost parameter. The operating costs are made up of input fresh resources IF_r the fixed and variable operating cost of process $pa_o_p^{variable}$ and ao_p^{Fixed} respectively. It should emphasize that, the CAPEX term in the objective function is user specified. Therefore, the CAPEX of existing plant can be equaled to zero.

It is noteworthy that the model is subjected to a number of constraints which can be demand constraints, fresh feed constraints, or resource output constraints. Demand constraints can be fulfilled by production facilities, fresh feed and resource output constraints are restricted by the minimum and maximum feed allowed. The mathematical form of these constraints can be found as below.

The capacity (C_p) was constrained between minimum (C_p^{min}) and maximum limits (C_p^{max}):

$$C_p^{min} \leq C_p \leq C_p^{max} \quad (2)$$

Resource flow rate constraints between minimum (IF_r^{min}) and maximum (IF_r^{max}) flow limits.

$$IF_r^{min} \leq IF_r \leq IF_r^{max} \quad \forall r \in R \quad (3)$$

Non-negativity constraints:

$$IF_r \geq 0 \quad \forall r \in R \quad (4)$$

4. Case Study

The proposed approach was applied to an industrial cluster tasked to produce hydrogen accounting for economic cost and environmental impact. The cluster is to produce sustainable and low-cost 30,000 t/y of hydrogen and to utilize CO₂ that emitted from the cluster to produce added-value products given options of Methanol, Ammonia, and Urea production. In the proposed cluster, natural gas is the only hydrocarbon to be allowed as input along with seawater and air. The treated CO₂ is processing through possible technologies namely the Methanol process, urea process as well as sequestration process in which the compression and injection into the geographical formation of the CO₂ take place. Various possible technologies are selected for hydrogen production, SMR, Water electrolysis, and Kvaerner. For the power supply, a conventional power plant (gas-fired power station), as well as a photovoltaic power station, are included to generate the required electricity. Seawater Reverse Osmosis (SWRO) is selected for freshwater supply. An Air separation Unit (ASU) is selected to enable the separation of air into O₂ and N₂ for ammonia production. The price of the resources included in the cluster is obtained from Ahmed et al (2020) as well as the economic data (e.g., CAPEX and additional OPEX) are given in Table 1. CAPEX and additional OPEX of Methanol, Ammonia, Urea, and ASU are obtained from Ahmed et al (2020). SWRO Plant CAPEX is estimated from the database given in (World Bank, 2019). Economic data for the gas-fired power station is obtained from Al-Mohannadi et al (2017). PV CAPEX data is obtained from Sargent & Lundy LLC (2020). The capital cost for CCS as well as CO₂ sequestration was obtained from Ahmed et al (2020).

Table 1 Summarizes the economic data as well as the resource price in /t, otherwise mentioned

Plant	Resource	Resource price (\$/t)	CAPEX (\$/t Ref)	Additional OPEX (\$/t Ref)
SMR	CH ₄	136	340	-
	H ₂	1,000		
Water Electrolysis	O ₂	100	830	-
	H ₂	1,000		
Ammonia	NH ₃	415	29.17	-
Methanol	CH ₃ OH	320	21.46	-
Urea	CO(NH ₂) ₂	305	16.11	7.71
Methanol CCS	-	-	1.70	5.28
Urea CCS	-	-	1.70	5.28
CO ₂ sequestration	-	-	9.02	-
ASU	-	-	18.16	-
NG Power plant	-	-	1,000 \$/kW	-
PV power plant	-	-	1,313 \$/kW	-
SWRO	-	-	2	-

4.1 Results and discussion

The problem was solved by using LINDO "What'sBest! 17.0" solver (LINDO, 2020) to obtain the optimum network configuration by taking into account the economic performance as well as environmental performance

The results of the two cases are presented in this section. In the first case (Case A), it was found that when the cluster network was restricted to export hydrogen of 30,000 ton/y and no environmental restrictions were imposed, the model activated natural gas-fired power plant, SWRO plant, and SMR. The visual representation of this case is depicted in Figure 1. Setting the hydrogen selling price at \$1 /kg H₂, the optimized network achieved an annual profit of about \$34 million, and total emissions of CO₂ 249k t/year, while the total cost is maintained at \$2.49 /kg H₂ without by-products revenues. It is noteworthy to highlight that the model did not activate the water electrolysis plant, and this was attributed to the higher capital cost of water electrolysis. The model activates Natural gas-fired power plant to satisfy the power requirement of the cluster, whereas PV-powered water electrolysis activation in comparison will attribute to lower profit. The model activates Ammonia to be utilized as a feedstock in urea production as it will result in higher profit. The methanol plant activation will be led to more cost as the CO₂ emissions restrictions were not imposed.

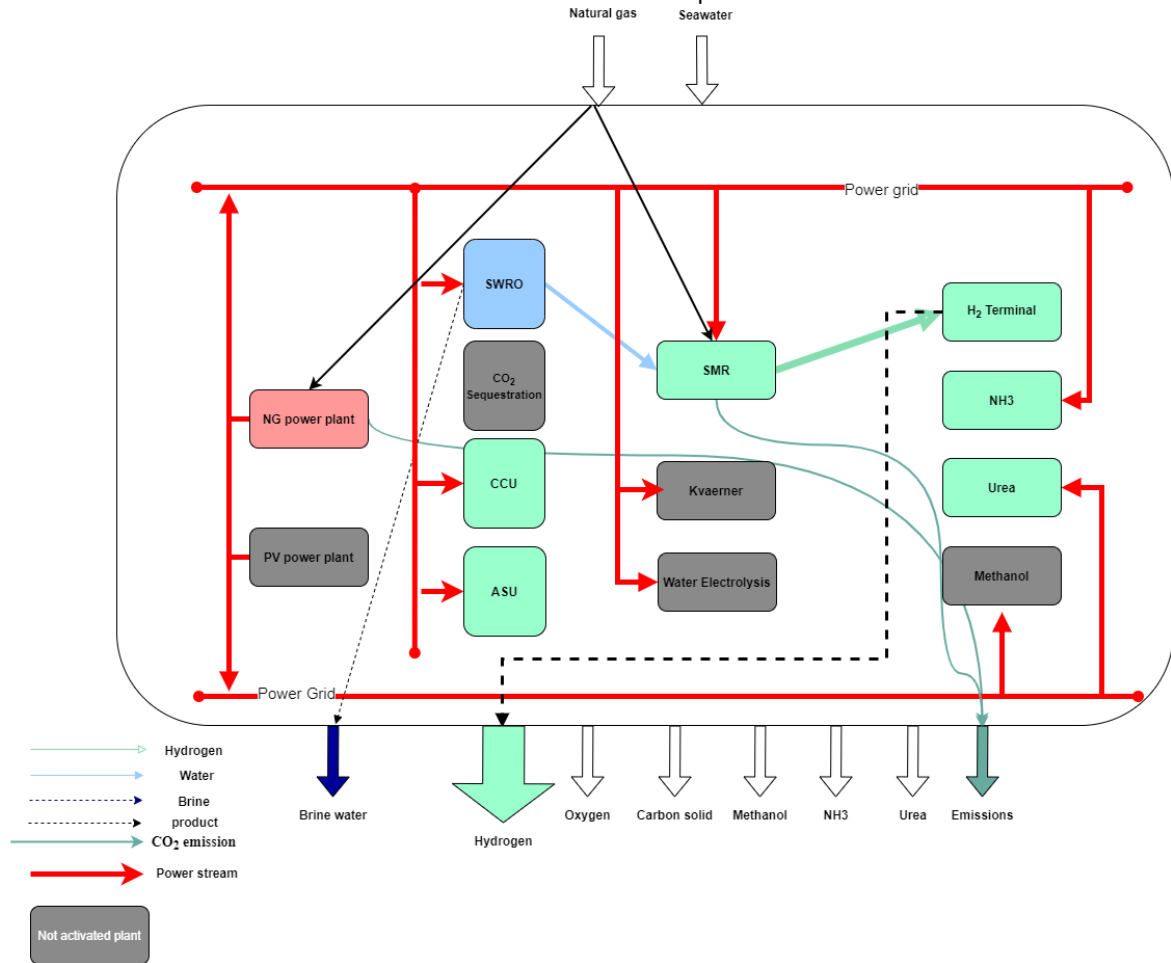


Figure 1: Case-A Network

In case B where the CO₂ emissions reduction protocol is set to different targets. Each set of goals for CO₂ reduction with the same H₂ selling price as in case A yields to different optimal hydrogen network designs. At 60 % CO₂ reduction protocol the optimized cluster still maintained an annual profit with a significant drop about 90 % less than in the first case (\$ 3 million). However, the trade-off between the cost and emissions reduction protocol gains is observed since the CO₂ emissions is reduced up to 99.5k ton of CO₂ annually, while the total cost without by-products revenues increased to \$2.88 /kg H₂. The visual representation of the proposed network is shown in Figure 2. The allocation of hydrogen and treated CO₂ shifts to mitigating CO₂ emissions and to produce added-value products. The profitability of this case can be attributed to the return revenues from selling these added-value products which in this case is methanol and oxygen. In addition to maintaining the exporting hydrogen capacity as in the first case without any reduction. The activation of methanol was found to be more cost-effective and contributes to more revenue. It can be noted that the emissions reduction protocol has led to incorporate the green hydrogen through PV-powered water electrolysis and hydrogen supplied from the

Kvaerner plant to satisfy the hydrogen export constraints. It is noteworthy that the model did not activate ammonia and urea due to the higher production cost that results from activating these plants.

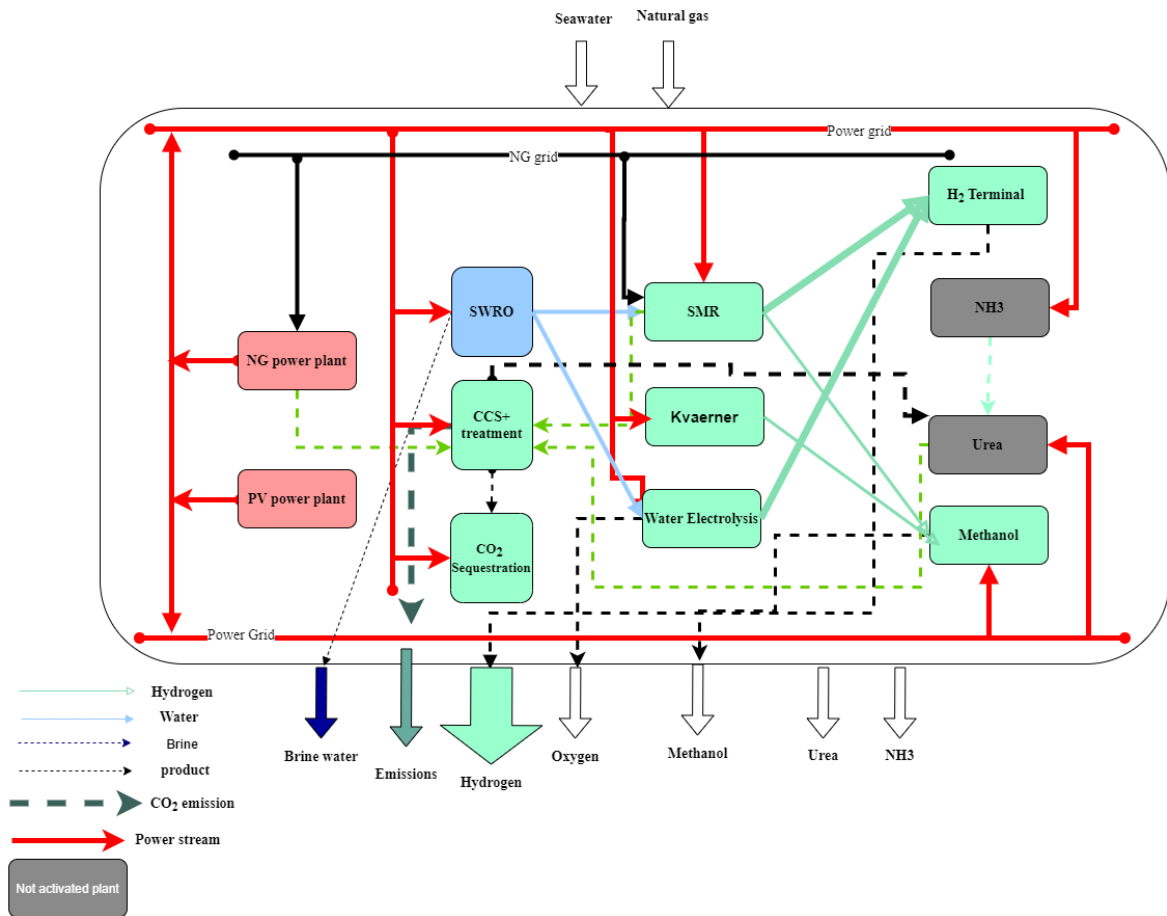


Figure 2: Case-B Network

5. Conclusion

A MILP model formulation was formulated based on the prescribed method to enable the simultaneous exploitation of hydrogen and CO₂ utilisation options to identify the optimum network design that helps to yield the maximum total profit that can be extracted from the proposed cluster whilst being in the range of allowable CO₂ footprint. Two case studies where it is assumed there are no environmental constraints and with environmental constraints were developed to investigate the applicability of the proposed method. As a first insight, the proposed network experienced a significant change in the design configuration as the environmental restrictions were imposed. The profitability of the network under CO₂ restriction as in case B can be attributed to additional revenue that was achieved from utilizing hydrogen and CO₂ to produce more products. It was found that the fuel price is the key operating parameter that has a major impact on the cluster network design. Taken together, this model presented in this work has several important implications towards linkage between the competing hydrogen supply pathways and the demand for clean and affordable hydrogen in order to pave the way for policymakers in drafting global energy solutions.

Notwithstanding, further comprehensive and coherent modelling work will have to be conducted in order to address the inherent interconnection as well as the spatial characteristics of the hydrogen supply chain network. Therefore, this can be done through 1) examining various hydrogen storage alternatives and associated costs; and 2) investigating the cost of different alternatives to distribute hydrogen locally and for long-distance transmission (i.e., offshore hydrogen distribution).

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