

A Techno-Economic Optimization Approach to an Integrated Biomethane and Hydrogen Supply Chain

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ABSTRACT

One of the proposed strategies to reach net-zero goals is the diversification of a country's energy mix and transition to technologies that favour the mitigation of greenhouse gas emissions, while decreasing dependency on conventional fuels. This work presents a mathematical model that describes key production routes for two proposed energy transition vectors, biomethane and hydrogen, expressed as a Mixed-Integer Linear Problem (MILP). The supply chain is optimized with the objective of maximizing the profits from the global supply chain. The problem is formulated as an allocation problem, with production distributed between biomethane and hydrogen markets. The case study focuses on a region in Mexico where second-generation biomass for biogas production is abundant, while hydrogen is produced from biomethane using steam methane reforming. The results highlight the importance of balancing resource allocation in shared supply chains. With a production ratio of 60% biomethane and 40% hydrogen, a Levelized Cost of Hydrogen (LCOH) of 2.07 €/kWh and a Levelized Cost of Biomethane (LCBM) of 0.17 €/kWh are obtained, resulting in total hydrogen and biomethane production of 12,563 GWh/year and 72,374 GWh/year, respectively.

Keywords: Optimization, Environment, Hydrogen, Renewable and Sustainable Energy, Supply Chain

1. INTRODUCTION

A country's energy consumption is closely linked to its economic growth. Despite efforts to reduce greenhouse gas emissions by integrating green technologies to meet energy demands, energy consumption remains heavily reliant on fossil fuels. On a global scale, oil and gas production is projected to increase by 27% and 25% by 2030 [1]. According to the findings of the Intergovernmental Panel on Climate Change (IPCC) in 2018, limiting global temperature rise to no more than 1.5°C requires nations worldwide to achieve net-zero emissions by 2050 [2]. To reach this goal, different pathways have been proposed, which include the use of various technologies to decarbonize hard-to-abate sectors [3]. These sectors, which account for 30% of global emissions, encompass industry applications such as cement, plastics, and steel, as well as heavy-duty transport. Among the proposed technologies for decarbonization, biomethane and hydrogen have emerged as promising solutions,

supported by the extensive research into their production technologies and associated limitations. Biogas is obtained from organic waste, and its process occurs naturally in landfills when it decomposes and produces methane, which is twenty times more damaging to the atmosphere than carbon dioxide [4]. Hydrogen production is currently dominated by steam methane reforming (SMR) using natural gas. Since SMR is a well-established technology, using biomethane obtained from biogas offers an attractive alternative for hydrogen production [5]. The use of biomass for methane and hydrogen production fosters a circular economy by reincorporating waste into the value chain [6], significantly reducing greenhouse gas (GHG) emissions. Waste-to-energy systems provide dual benefits: improved waste management and enhanced energy security, as the production and consumption of the resulting product can be located within the same geographic region. To address some of the challenges that arise from the network design of these technologies, various approaches have been proposed.

For instance, the application of a multi-objective optimization approach for biogas supply chains that considers the upgrading of biogas to biomethane reduces environmental impact and enhances applicability to different end-users. However, this also leads to higher production costs [7]. Additionally, some studies have considered inorganic waste sources to obtain a range of products in addition to electricity, such as syngas [8], incorporating the minimization of GHG emissions. A key advantage of biogas production is its feedstock flexibility, making it a more reliable energy source compared to the inherent variability of wind and PV energy [9]. In parallel, there is extensive research on hydrogen supply chains [10-12], which determines key components for the optimal supply chain design (energy source, production technology, storage, transportation, end-use). For green hydrogen production, the prominent technology used is electrolysis, relying on electricity production from renewable energy sources (RES). However, production costs and availability are highly dependent on the geographical region. Some frameworks have been developed to integrate dual product demands within a single supply chain network, such as hydrogen and methane through Power-to-Hydrogen (which transforms energy into hydrogen) and Power-to-Methane concepts (which produces methane through methanation) [13]. These approaches aim to provide fuel supply at a lower carbon-cost, while mitigating the impact from RES fluctuations. In the present study, biomethane and hydrogen are considered as products from a shared supply chain, which uses second generation waste as biomass source, a strategy particularly relevant to avoid the use of energy crops. Biogas is produced through anaerobic digestion and subsequently upgraded to biomethane. Hydrogen is generated via SMR, with biomethane being allocated between market demand and hydrogen production based on a specified distribution ratio. The interdependency of these products is analysed using a techno-economic approach through a set of equations that consider resource allocation and distribution, as well as cost constraints.

1.1 Methodology

The framework for the techno-economic assessment for biomethane and hydrogen production consists of three steps. First, the potential biomethane and hydrogen markets are analysed, considering the demand for each product. In the case of biomethane, its use in the domestic sector and electricity production sector is considered. Two hard-to-abate sectors are identified for hydrogen: the heavy-duty transport sector and the steel sector. The second step comprises the formulation of the mathematical model, which is based on the superstructure shown in **Figure 1**. Finally, the supply chain is optimized considering the maximization of global profits as the objective function.

The mathematical model incorporates mass balance equations in a steady-state configuration. The supply chain considers the following echelons: biomass is obtained from location f and processed into biogas using technology j in location l . Biofertilizer is obtained as a by-product and can be sold in demand market q . Biogas is upgraded using technology k in location m . The upgraded biogas, or biomethane, is sold at demand market p . Biomethane that is not sent to the demand market p is used to produce hydrogen, which is produced using technology r . As this results in gaseous-state hydrogen, a liquefaction step is needed, using technology lq , to store liquid hydrogen in storage tank s and to be able to transport it in liquid form to location h , where it is regasified to be distributed through the refuelling station rf . The mathematical model is formulated as a mixed integer linear programming model (MILP). Since this is a preliminary assessment, uncertainty in the process was not considered. The supply chain is modelled as an allocation problem, where a percentage of the obtained biomethane will be sold to the demand market and the other percentage is used to produce hydrogen.

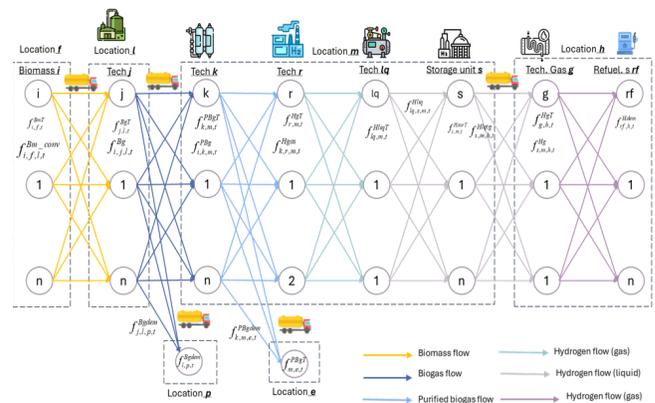


Figure 1. Proposed superstructure for the biomethane and hydrogen supply chain.

2. MATHEMATICAL MODEL

2.1 Biogas and Hydrogen Production

The total amount of biomethane ($f_{k,m,t}^{PBg-T}$) using technology (k) at location (m) must be equal to the sum of biogas from every biomass source (i) purified at location (m) using technology (k). It should also be equal to the amount of biomethane ($f_{k,m,p,t}^{PBg-market}$) needed to satisfy market (p) and the amount of biomethane allocated for hydrogen production ($f_{k,m,t}^{BGH}$).

$$f_{k,m,t}^{PBg-T} = \sum_i f_{i,m,k,t}^{PBg}, \forall (k \in K, m \in M, t \in T) \quad (1)$$

$$f_{k,m,t}^{BGH} = x \sum_i f_{i,m,k,t}^{PBg}, \forall (k \in K, m \in M, t \in T) \quad (2)$$

$$f_{k,m,t}^{PBg,T} = \sum_p f_{k,m,p,t}^{PBg,market} + \sum_i f_{i,m,k,t}^{Bgh}, \forall (k \in K, m \in M, t \in T) \quad (3)$$

The balance in the storage unit *STOR* of type *s* in location *m* at time *t* is given by the difference between the flows that go into the storage unit and the mass flows leaving the storage unit.

$$STOR_{s,m,t} = STOR_{s,m,t-1} + \sum_{lq} f_{lq,s,m,t}^{Hliq} - \sum_h f_{s,m,h,t}^{Hlqrf} \quad \forall (s \in S, m \in M, t \in T) \quad (4)$$

To make sure that the liquid hydrogen flow to and from the storage unit *u* at production site *m* during time *t* is within the storage unit capacity limit, the following restriction is applied:

$$SCap_{s,m,t}^{\min} \cdot \gamma_{s,m}^s \leq STOR_{s,m,t} \leq SCap_{s,m,t}^{\max} \cdot \gamma_{s,m}^s \quad (5)$$

$SCap_{s,m,t}^{\min}$ and $SCap_{s,m,t}^{\max}$ represent the minimum and maximum storage capacities for the storage tank type *s* at location *m* in time *t*.

2.2 Economic objective

The total profit (*Pft*) considers the revenue (T_Rev) obtained from sales for each product minus the total costs from the supply chain, which include fixed costs (T_FC), variable costs (T_VC), and transport costs (Tr_C).

$$Profit = TotalRevenue - TotalCosts \quad (6)$$

The fixed costs (*FC*) for each process *X* involved in the supply chain are calculated by multiplying the annualization factor *K* by the parameter *CF* and the binary variable *y*, which dictates whether the process technology *X* will be installed or not.

$$FC[processX] = KX_{x,t} \cdot CF_{x,t} \cdot y_{x,t} \forall t \quad (7)$$

The annualization factor *K* is calculated as follows:

$$k_{x,t} = \left[\frac{(1+\alpha_x)^n \cdot \alpha_x}{(1+\alpha_x)^n - 1} \right] \quad (8)$$

In this expression, *x* refers to the production technology, α is the discount rate set at 10%, and *n* is the plant lifetime (20 years). The variable costs are computed by the product of the parameter *VC* by the mass flow relevant to the conversion process at each stage. For instance, considering the SMR process, the parameter $VC_{m,r,t}^{ref}$ is multiplied by the mass flow $f_{k,m,r,t}^{Hgas}$, that is used for hydrogen production.

$$VC^{ref} = \sum_k \sum_m \sum_r \sum_t CV_{m,r,t}^{ref} \cdot f_{k,m,r,t}^{Hgas} \quad (9)$$

Transport costs consider fuel, labour, and maintenance costs, multiplied by the demand flows, taking into account the distance between the production site and the demand market. The total costs are the sum of the fixed,

variable, and transport costs.

$$TotalCosts = Total_{FC} + Total_{VC} + Total_{TR} \quad (10)$$

Finally, the levelized costs for biomethane and hydrogen respectively *LCOH* and *LCBM* are calculated as follows:

$$LCOH = \frac{Total\ hydrogen\ production\ costs}{Annual\ hydrogen\ production} \quad (11)$$

$$LCBM = \frac{Total\ biomethane\ production\ costs}{Annual\ biomethane\ production} \quad (12)$$

The mathematical model is expressed as a Mixed-Integer Linear Problem (MILP). This was solved using CPLEX 22 within the GAMS environment. The model consists of 83 blocks of equations and 70 blocks of variables. The supply chain is optimized with the objective of maximizing the profits from the global supply chain. The problem is expressed as an allocation problem, with production distributed between biomethane and hydrogen markets.

3. CASE STUDY

The mathematical model is applied to a case study in Mexico, focusing on the country's central region. The states selected play a significant role in the agricultural sector, resulting in a high availability of residues that can be used as feedstock for biogas production. For market demands, biomethane is considered a substitute for natural gas in energy production. Regarding hydrogen, market trends in Mexico highlight its potential to decarbonize the heavy-duty transport sector and some hard-to-abate industries, such as steel and ammonia production. In this case study, the heavy-duty transport sector was considered. GHG emissions from road transportation in Mexico contribute to 34% of the total emissions [14]. With current tendencies suggesting increased investment in the industry sector in the country, this number is expected to grow even further.

4. RESULTS

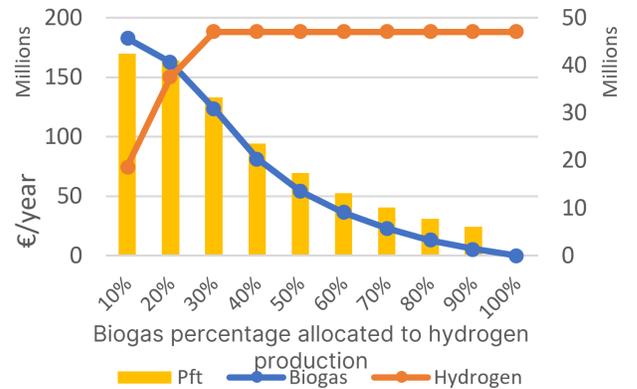


Figure 2. Revenue per product

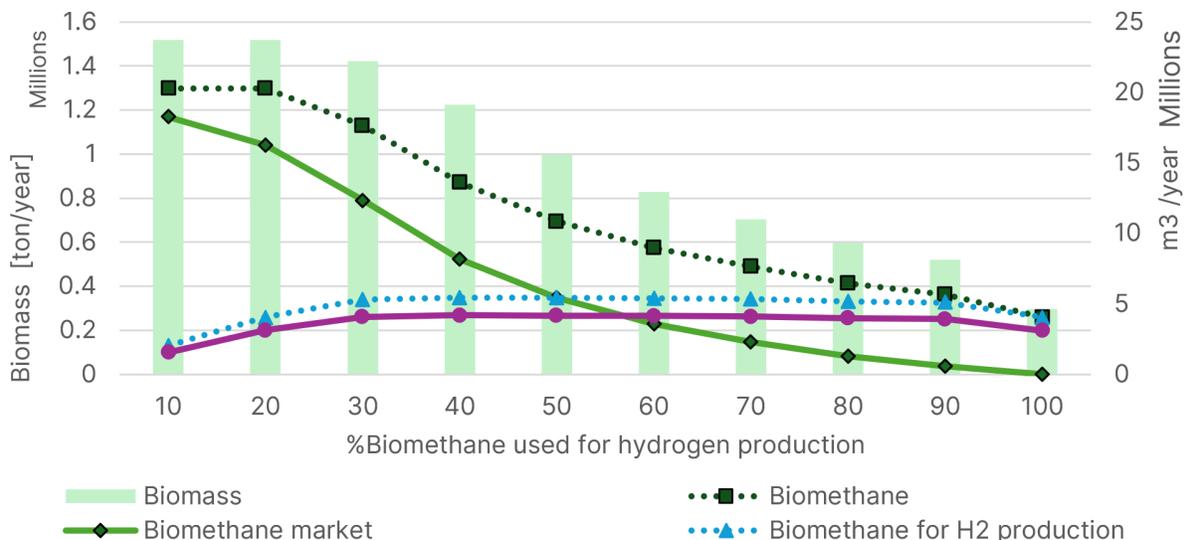


Figure 3. Impact of Biomethane Allocation on Hydrogen and Biomethane Production.

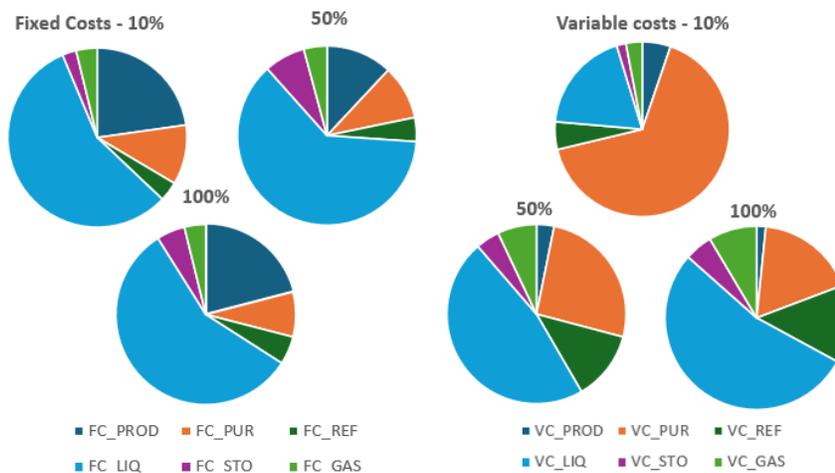


Figure 4. Share of Fixed and Variable costs.

Figure 2 illustrates a clear trend, showing the profit for each allocation scenario. As the quantity of biogas allocated to hydrogen production increases, profits decrease significantly. Biomethane revenue decreases as the amount of biomethane allocated for hydrogen production rises, which aligns with the concept of economy of scales. This concept refers to the cost advantages with the increase in production. However, hydrogen revenue remains constant, from 30% of biomethane allocation for hydrogen production onwards. The main reason for this trend is the inflated cost of hydrogen production, specifically, its liquefaction, which is a crucial step needed to store and transport from the production site to refuelling stations.

This is further demonstrated in **Figure 3**, which shows that with a higher percentage of biomethane being used for hydrogen production, the overall of biomass required for the supply chain is adjusted to maintain

profitability. This decrease helps in controlling costs associated with hydrogen production. As it can be observed in **Figure 4**, when hydrogen is produced from 10% biomethane, the fixed costs for the liquefaction technology take up more than half of the overall capital costs. This contribution remains constant up to the point where all biomethane is used to produce hydrogen. Yet, in terms of operational costs, the main contributor is the cost from upgrading biogas to biomethane. As hydrogen production increases, these costs become negligible compared to those associated with hydrogen liquefaction.

Figures 5 and 6 present the levelized costs in terms of energy, considering that 1 m³ of biomethane and 1 m³ of hydrogen gas have a Low Heating Value (LHV) of 10 kWh/m³ [15] and 3 kWh/m³ [16], respectively. Under these assumptions, the highest LCBM for this supply chain reaches 1.04 €/kWh, while the highest LCOH amounts to 5.06 €/kWh. In **Figure 5**, an exponential trend

is noticeable from allocating 40% to the biomethane market onwards. Since the revenue from biomethane is higher than that from hydrogen, the optimization strategy seeks to limit its production. Considering the LCOH (**Figure 6**), this value decreases as more biomethane is used in production but stabilizes between 2€/kWh to 1.6€/kWh from scenario D onwards, maintaining a constant profitability in the system.

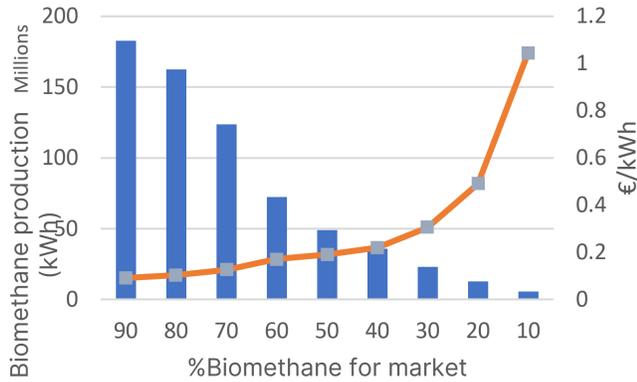


Figure 5. Levelized cost of biomethane (LCBG)

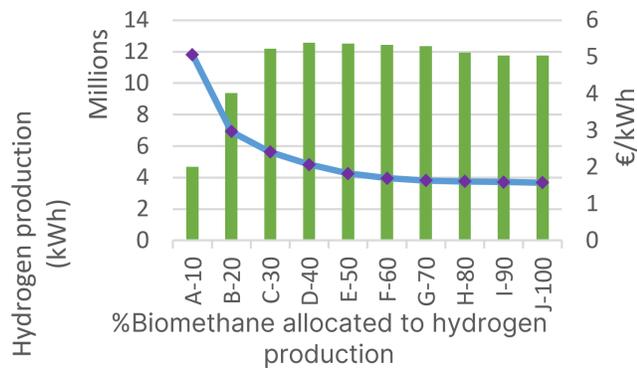


Figure 6. Levelized cost of hydrogen (LCOH)

Figure 7 provides a schematic representation of the supply chain design resulting from scenario “D”, covering six of the most industrialized and energy-driven cities (labelled 1 to 6). The network integrates biogas upgrading, hydrogen production, transport, and refuelling infrastructure to support a sustainable energy transition. In this scenario, 1,224,103 tons of biomass are collected at each of the locations, consisting of 3% from organic waste, 11% from cow manure, and 86% from wastewater. To maintain profit margins, biomass is obtained, transformed to biogas and upgraded to biomethane within the same locations where biomethane is distributed. The upgrading technology used to produce biomethane is High-Pressure Water Scrubbing (HPWS), obtaining 8,173,563 nm³ of biomethane to be sold to the demand market, while 4,8249,93 m³ are used to produce hydrogen by SMR, representing a 60-40 ratio. From this configuration 4,187,805 m³ of hydrogen are regasified at the refuelling stations. Hydrogen production plants, storage, and

refuelling stations are installed at all locations, and hydrogen distribution prioritizes the demand of the most industrialized cities, locations 1 and 6. The LCBM presents a value of 0.17 €/kWh, while the LCOH is 2.07 €/kWh.

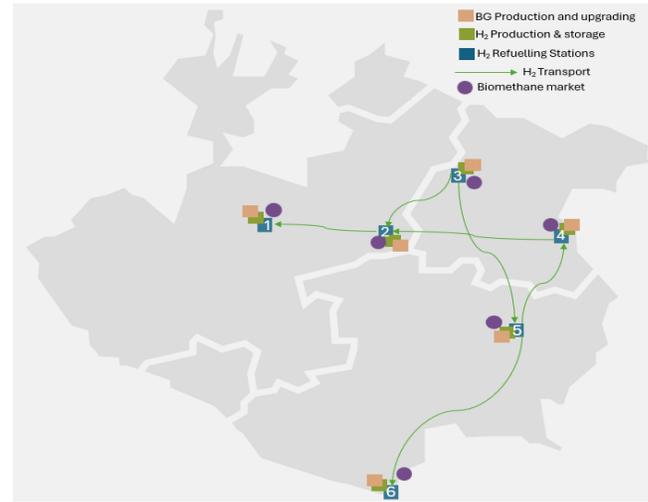


Figure 7. Supply chain design for scenario “D”.

5. Conclusions

The techno-economic optimization for a biomass and hydrogen supply chain is considered for a case study in Mexico. The objective function is profit-maximization of the global supply chain. It is well-established that hydrogen production is an expensive process, compared to biomethane production. Therefore, the optimization problem is formulated as an allocation problem, to distribute the quantity of biomethane that is used for hydrogen production. These results emphasize the importance of balancing resource allocation in shared supply chains. A production scenario with 60% biomethane and 40% hydrogen offers a balanced cost-effectiveness for both products with a LCOH of 2.07 €/kWh and an LCBM of 0.17 €/MWh, with total hydrogen and biomethane production of 12,563 GWh/year and 72,374 GWh/year, respectively. While the LCBM is slightly higher than average LCOE for biomethane (0.1 €/MWh [17]), the hydrogen costs are quite further from average LCOH costs in literature. This can be explained by the relatively low demand for hydrogen considered for this case study. However, costs can be reduced through government subsidies, carbon taxes to incentivize the use of cleaner energy sources, as well as considering the optimization of energy-intensive processes. Furthermore, there is a need to conduct an environmental evaluation of the supply chain to assess the impacts of these products on various environmental indicators. One key indicator is water use throughout the supply chain, as water is required at multiple stages, including biogas production in digesters, upgrading biogas to biomethane, and hydrogen production. The comparison between producing hydrogen from biomethane

through SMR, and producing green hydrogen through electrolysers, which relies on fresh water, is a critical consideration, particularly in water-stressed regions. The use of life cycle assessment to evaluate this (and other) environmental indicators will further allow the evaluation of the supply chain from a multi-objective perspective and enrich the discussion of the integration of these technologies, while ensuring compliance with energy policies and sustainability goals.

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