A Bilevel Framework for Environmental and Economic Optimisation of Hydrogen Supply Chains

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Abstract

Hydrogen is an energy carrier with the potential to decarbonise a portion of the transportation sector. To achieve this, there is a need to deploy a whole supply chain to produce, transport, store, and distribute this low-carbon fuel. Although hydrogen can be low-carbon if produced via the electrolysis of renewable electricity, most of its current production relies on fossil resources such as natural gas. It is thus crucial to develop a hydrogen supply chain that combines the reduction of greenhouse gas emissions to decarbonise mobility with the optimization of economic objectives. Most of the frameworks that model the hydrogen supply chain (HSC) with associated greenhouse emissions use a multi-objective approach to account for it. The whole supply chain is considered as a single actor with the goal of minimising both the total cost and the greenhouse gas (GHG) emissions of the HSC. This paper proposes a new approach involving two stakeholders with competing objectives. The problem is modelled as mixed-integer bilevel programming problem (MIBLPP) including a decision-maker with the aim to minimise GHG emissions as the upper level (UL) and the minimisation of the total cost of the HSC at the lower level (LL). The UL can choose technologies to subsidise in order to support the greenest solutions, while the LL will design the most cost-effective HSC to fulfil the demand based on the availability of technologies and energy sources.

**Keywords**: Hydrogen Supply Chain, Optimisation, Bilevel, MILP, Evolutionary Algorithm.

* 1. Introduction

The Paris Agreement sets the goal of maintaining “the increase in the global average temperature to well below 2°C above pre-industrial levels” and further aims “to limit the temperature increase to 1.5°C above pre-industrial levels”. To achieve this, participating countries have to cut down their greenhouse gas emissions. According to the French High Council on Climate (HCC), the transport sector was the main source of GHG emissions, accounting for 31% of France's total emissions in 2021 (HCC, 2021). To decarbonise this sector mainly driven by fossil fuels, various technical solutions are being explored, including batteries, biofuels or green hydrogen. The latter refers to hydrogen produced from renewable energy sources, in contrast to grey hydrogen which is fossil-based. Hydrogen is mainly used to produce electricity with fuel cells, powering electric engines

However, for hydrogen to serve as a solution for decarbonising mobility, a whole supply chain is required. This hydrogen supply chain is composed of production plants, hydrogen transport facilities, storage units and distribution stations. The literature review highlights that the predominant engineering model of such energy systems involves a mixed-integer linear programming (MILP) approach (e.g., Almansoori and Shah, 2009 and De-León Almaraz et al., 2014). This modelling approach determines the optimal HSC to satisfy an objective function such as cost minimisation or GHG emissions reduction through cooperation among stakeholders. However, real-world HSC design and management often encompass multiple actors across the different levels, ranging from production to distribution. These challenges involve a hierarchical relationship between two decision levels and are generally formulated as mixed-integer bilevel programs (Bard 1998).

This paper addresses this issue by taking into account the constraint of renewable energy availability in the territory to be considered for hydrogen production and the investment choices for new facilities. To tackle this problem, we propose a bilevel framework using an evolutionary algorithm at the upper level (leader) to select the most consistent subsidies for minimising the total GHG emissions. The lower level (follower) involves a mixed-integer programming formulation to minimise the cost of hydrogen production, transport, storage and distribution based on the model developed by De-León Almaraz (2014). We then apply our methodology to model and optimise an HSC in a sub-area of the Occitanie region in France. The proposed framework has the potential to aid in determining regulations and economic instruments for deploying low-carbon based hydrogen supply chains. Additionally, it allows for the consideration of the impact of policymakers’ decisions on the optimal configuration of the HSC.

* 1. Definition of the MIBLPP model
     1. Structure of the algorithm

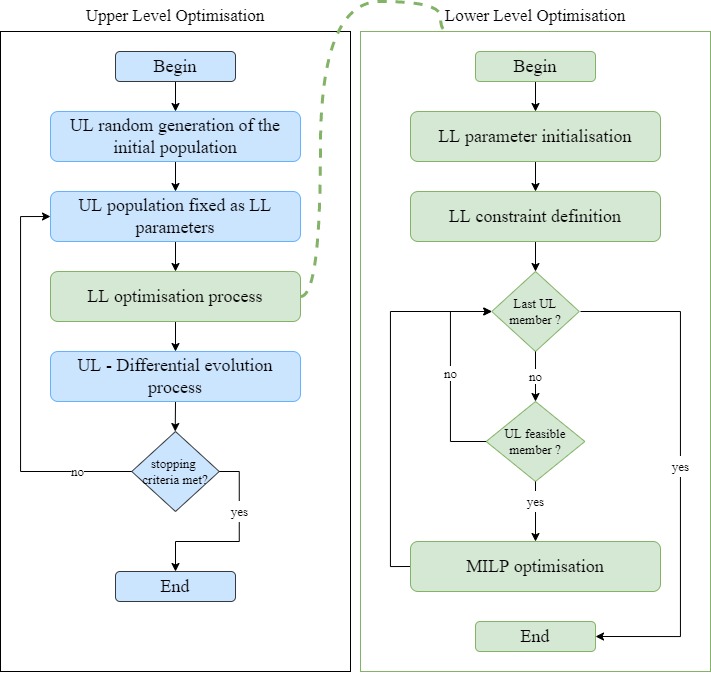
The algorithm designed to model the HSC deployment was implemented using the Python programming language and involves a mixed-integer bilevel programming approach. The

Figure 1: Structure of the MIBLPP algorithm

LL (follower) replicates the approach defined by De León Almaraz et al. (2014) to model the technical aspects of the HSC which is formulated as a mixed-integer linear programming (MILP) problem. It minimises the total cost of the HSC based on the hydrogen demand and techno-economic parameters. The LL also calculates the GHG emissions of the entire supply chain (expressed in kgCO₂eq). To transfer the previously designed GAMS (General Algebraic Modelling Language) model to Python, the algebraic modelling language Pyomo (Python based) was used. The UL and the structure of the MIBLPP algorithm are based on the work by Flores-Perez et al. (2020) and Avraamidou and Pitsikopoulos (2019). Figure 1 describes the framework designed to model this MIBLPP. The UL fixes the UL variables (i.e., binaries for the choice of technology or energy sources to subsidise) of each population member and sends them to the LL as parameters. The LL is solved with Gurobi solver and the results are used to calculate the UL objective function. A differential evolution is then performed to generate new population members for the next iteration. For more details on the Python MIBLPP framework, see Jacquot et al. (2023).

* + 1. Formulation of the mathematical equations

Eqs. (1-3) describe the UL that minimises the total CO₂ emissions (Eq. 1). The model can choose to subsidise renewable energies or electrolysers procurement (Eq. 2). Eqs. (4-10) are the main equations used by the LL. The objective is to minimise the total operating and investment cost (Eq. 4). Eq. (5) ensures that the level of production or storage respects the maximum and minimum capacities of facilities. The quantity distributed in each portion of the territory (or grid) (Eq. 7) must satisfy the demand (Eq. 8). The subsidies granted by the UL are applied to the units’ production costs (Eq. 8) and the plants’ capital costs (Eq. 9). Eq. (10) calculates the total CO₂ emissions for the production, storage and transportation of hydrogen (see Table 1). For more details on the equations used by the LL, see De León Almaraz (2014).

Table 1: Sets, parameters and variables

|  |  |
| --- | --- |
| Sets and index |  |
| F, f | Set of facilities (production, storage) |
| G, g | Set of grids |
| E, e | Set of primary energy sources |
| Parameters |  |
| Capmin, Capmax | Minimum and maximum capacities of facilities (kg/day) |
| Demand | Daily hydrogen demand in each grid (kg/day) |
| sub | Rate of subsidy |
| UPC | Hydrogen production cost ($/kg) |
| USC | Hydrogen storage cost ($/kg/day) |
| PCC | Investment cost of a production plant ($) |
| SCC | Investment cost a storage unit ($) |
| A0 | Available primary energy in each grid (GJ/day) |
| Variables |  |
| x | Binary of choice for subsidising energy purchase |
| y | Binary of choice for subsidising electrolysers purchase |
| FOC | Facility operating cost ($) |
| TOC | Transport operating cost ($) |
| CEC | CO₂ emissions cost (due to carbon tax) ($) |
| FCC | Facility capital cost ($) |
| TCC | Transportation capital cost ($) |
| Q | Quantity of hydrogen distributed, produced, imported, exported (kg/day) |
| GWP | Global warming potential of HSC (kgCO₂eq.) |

|  |  |
| --- | --- |
|  | (1) |
|  | (2) |
|  | (3) |
|  | (4) |
|  | (5) |
|  | (6) |
|  | (7) |
|  | (8) |
|  | (9) |
|  | (10) |

* 1. Case study

To illustrate this model, we propose a case study on the deployment of the HSC in a sub-area of the Occitanie region in France. Three geographical zone is discretized with an independent demand in each grid: the three grids considered correspond to the departments. The production technologies involved are steam methane reforming (SMR) and electrolysis from wind, photovoltaic, hydraulic, and national grid electricity. Hydrogen is stored and transported in its liquid form. Most of the data used come from the work of De-León Almaraz (2014) and Mashi et al. (2023). Table 2 summarises some of the parameters considered for the case study. SMR is identified as the cheapest technology albeit with the highest CO₂ emissions, and carbon capture technology is not included in this study. In this scenario, investment costs for electrolysers and SMR plants are assumed to be similar (Hecht and Pratt, 2017). Electrolysers can only operate with the primary energy available in their grid, whereas SMR units rely on imported natural gas. A single period of twenty years is considered, with a constant daily demand (see Table 2). A discount rate of 5% is applied to discount costs over time.

Three scenarios for producing low-carbon hydrogen (i.e., hydrogen with a carbon intensity lower than 3 kgCO₂eq./kgH₂) are compared: subsidies only, carbon tax only and a hybrid approach combining subsidies, and carbon tax.

Table 2: Parameters of the case study

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  |  | PV | Wind | Hydraulic | Electrical grid | SMR |
| UPC ($/kg) | Small | 7.25 | 6.89 | 8.67 | 5.28 | 2.21 |
|  | Medium | 7.04 | 6.68 | 8.44 | 5.13 | 1.82 |
| PCC (M$) | Small | 29 | 29 | 29 | 29 | 29 |
|  | Medium | 224 | 224 | 224 | 224 | 224 |
| GWPprod (kgCO₂eq./kgH₂) | Small / Medium | 3.08 | 0.984 | 1.68 | 2.15 | 10.3 |
| A0 (GJ/day) | g=1  g=2  g=3 | 1,196  1,440  1,335 | 533  1,751  1,114 | 106  20  228 | 43,835  43,835  43,835 | 0  0  0 |
| Demand (tH₂/day) | g=1  g=2  g=3 | 6.12  15.4  10.9 |  |  |  |  |

* 1. Results

This section presents the results found for the three scenarios of the case study. The scenarios incorporating subsidies rely on the MIBLPP algorithm previously described, while the scenario only involving a carbon tax is modelled using a conventional single level MILP approach. Table 3 shows the main key performance indicators (KPI) for each scenario compared to a reference scenario without GHG minimisation.

The MIBLPP opted to subsidise the procurement of renewable electricity instead of electrolysers, primarily due to its significantly higher total cost. Even if electrolysers were provided at no cost (unrealistic solution), SMR remains lower, because of the huge difference in primary energy costs. The subsidy needed for the transition away from fossil energies accounts for 95% of the electricity price. This substantial amount is attributed, in part, to the necessity of deploying two electrolysers (medium size, one per grid) as the available wind electricity in a single grid cannot satisfy the whole demand. With unlimited available electricity, a rate of 73% would be sufficient. While this scenario allows to decrease GHG emissions by 88%, it is noteworthy that the decision-maker bears more than half of the total cost.

The carbon tax scenario involves an electrolyser powered by the electrical grid because it enables the production of low-carbon hydrogen at a lower cost than with wind power. This scenario decreases GHG emissions by 77%, but with an 88% increase in the Levelized Cost of Hydrogen (LCOH). The decision-maker earns about 10% of the LCOH through carbon tax revenue.

The hybrid scenario results in the same production configuration as the first scenario with a reduction of 88% of GHG emissions. However, the carbon tax makes the SMR less profitable, leading to a 42% increase in the LCOH. The decision-maker will pay almost 40% of the total cost. To be more realistic, future work should encompass a broader geographical area, involving multiple grids, possibly an entire region. Additionally, this study should explore several different shorter periods and consider alternative technologies, such as SMR with carbon capture, as well as compressed hydrogen transportation and storage.

Table 3: KPIs of the case study

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Optimal values of the UL (in brackets) | Subsidies (95% of renewable electricity cost) | Carbon tax (420 $/tCO₂) | Subsidies (67% of renewable electricity cost) + tax (200 $/tCO₂) | Reference (no tax nor subsidy) |
| LCOH ($/kgH₂) | 3.05 | 5.72 | 4.35 | 3.06 |
| GWP (kgCO₂/kgH₂) | 1.21 | 2.37 | 1.21 | 10.5 |
| Tax ($/kgH₂) | 0 | 0.6 | 0.1 | 0 |
| Subsidy ($/kgH₂) | 3.9 | 0 | 2.8 | 0 |
| Production plants installed |  |  |  |  |
| g=1 | - | - | - | - |
| g=2 | 1 medium wind electrolyser | 1 medium grid electrolyser | 1 medium wind electrolyser | 1 medium SMR |
| g=3 | 1 medium wind electrolyser | - | 1 medium wind electrolyser | - |

* 1. Conclusions

This paper proposes an MIBLPP model for the HSC to help policymakers in making the optimal choices to minimise the GHG emissions of the HSC. The methodological framework includes an evolutionary algorithm to optimise the decision-maker’s choices and a MILP approach to optimise a multigrid HSC with investment choices. This approach allows for modelling the vertical relationship between two stakeholders of the HSC. Further work will focus on expanding the model to accommodate a more complex multiperiod HSC with new technologies and additional variables at the UL. To address horizontal competitive relationships and demand elasticity, a combined engineering-economic approach will be explored.

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References

A. Almansoori, N. Shah, 2009, Design and operation of a future hydrogen supply chain: Multi-period model, International Journal of Hydrogen Energy 34 (19), 7883–7897.

S. Avraamidou, E. N. Pistikopoulos, 2019, B-POP Bi-level parametric optimization toolbox, Computers and Chemical Engineering 122, 193–202.

J. F. Bard, 1998, Practical Bilevel Optimization, Vol. 30.

S. De-Leon Almaraz, 2014, Multi-objective optimisation of a hydrogen supply chain, INPT, Toulouse, France

S. De-Leon Almaraz, C. Azzaro-Pantel, L. Montastruc, S. Domenech, 2014. Hydrogen supply chain optimization for deployment scenarios in the Midi-Pyrénées region, France. International Journal of Hydrogen Energy 39 (23), 11831–11845.

J. M. Flores-Perez, C. Azzaro-Pantel, A. Ponsich, A. A. Aguilar Lasserre, 2020, A hybrid strategy for mixed integer bi-level optimization applied to hydrogen energy supply chain management, Modelling and Simulation 2020 – The European Simulation and Modelling Conference, ESM 2020, 277–281.

HCC, 2021, Rapport annuel du haut conseil pour le climat 2021 - Renforcer l’attenuation, engager l’adaptation.

E. S. Hecht, J. Pratt, 2017, Comparison of conventional vs. modular hydrogen refueling stations, and on-site production vs. delivery, Sandia National Laboratories, Albuquerque, New Mexico 87185 and Livermore, California 94550, U.S.A..

V. Jacquot, J. M. Flores-Perez, C. Azzaro-Pantel, S. Bourjade, C. Muller, 2023, Methods and tools for optimising supply chains modelled as mixed-integer bilevel programming problems, Modelling and Simulation 2023 – The European Simulation and Modelling Conference, ESM 2023, 375–382.

R. Mashi, Y. Vincotte, S. De-Leon Almaraz, C. Azzaro-Pantel, 2023, Optimization of Hydrogen Systems for Prospective Life Cycle Assessment: Well-to-Tank Approach, Computer Aided Chemical Engineering – 33 European Symposium on Computer Aided Process Engineering, Vol. 52, 3211–3217.