Multi-objective optimization of a hydrogen supply chain for vehicle use including economic and financial risk metrics. A case study of Spain

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Abstract
In this paper we present a decision-support tool to address the strategic planning of hydrogen supply chains for vehicle use under uncertainty in the operating costs of the network. Given a superstructure of alternatives that embeds a set of available technologies to produce, store and deliver hydrogen, the objective of our study is to determine the optimal design of the production-distribution network capable of fulfilling a predefined hydrogen demand. The design task is formulated as a multi-scenario mixed-integer linear programming problem (MILP) that decides on the production rates and expansions on capacity over time. The main novelty of the approach presented is that it allows controlling the variability of the economic performance of the hydrogen network at the design step in the space of uncertain parameters. This is accomplished by using a risk metric that is appended to the objective function as an additional criterion to be optimized. An efficient decomposition method is also presented in order to expedite the solution of the underlying mathematical model by exploiting its specific structure. The capabilities of the proposed modeling framework and solution strategy are illustrated through its application to a real case study based on Spain, for which valuable insights are obtained.

Keywords: Hydrogen, supply chain, mixed-integer linear programming, risk management, multi-objective optimization.

1. Introduction
The growing concern about possible disruptions in the oil supply and the need to reduce greenhouse gases (GHG) emissions have fostered in recent years the research for a more sustainable energy and transport model. In this context, hydrogen appears as a promising alternative fuel and energy carrier, since it can be produced locally, has the potential to be environmentally friendly and shows a wide range of applications [1]. Recent views suggest that the transition to the hydrogen economy will depend on two factors that must be developed in parallel: the construction of a hydrogen infrastructure has to be accompanied by policies promoting market for fuel cell technologies [1]. Focusing on the first of these factors, several mathematical programming models have been proposed that address the design of hydrogen supply chains (SCs). Most of these models are deterministic approaches assuming that all problem parameters can be perfectly known in advance. In the context of taking strategic decisions for developing a hydrogen infrastructure, this is an important limitation since the problem is in practice affected by different sources of uncertainty that can have a large impact on the final solution.
A possible way to overcome this limitation consists of applying stochastic optimization methods. Stochastic programming techniques allow assessing the performance of the problem under study in the space of uncertain parameters by optimizing the expected value of the objective function. In a more accurate way, financial risk metrics enable to take a step forward and control the variability of the objective function in the space of uncertain parameters [8]. Therefore, the introduction of a financial risk metric as an additional criterion to be optimized can be used to shape the form of the probability curves in order to reduce the possibility of having undesirable outcomes.

In the context of designing hydrogen SCs for vehicle use, only a few models have incorporated uncertainties [2, 3, 4], whereas none of them has applied financial risk management techniques. Hence, the aim of this paper is to consider the financial risk management associated with the long-term design and planning of hydrogen supply chains for vehicle use under uncertainty in production prices. The design task is posed as a multi-objective optimization problem where the expected total discounted cost of the network and a specific metric for financial risk (i.e. the worst case) are the objectives considered. The resulting large scale MILP tends to be computationally prohibitive as the number of time periods and potential locations for the SC entities increase. Hence, an efficient decomposition method is also presented to expedite the search for the Pareto solutions of the model by exploiting its mathematical structure. Finally, the capabilities of the proposed modeling framework and solution strategy are illustrated through its application to a real case study based on Spain.

2. Problem Statement

The design problem addressed in this paper has the objective of determining the configuration of a three-echelon hydrogen network for vehicle use (production-storage-market) with the goal of minimizing the expected total cost and financial risk. We consider a given region of interest (e.g., a country, a continent, etc.) that can be divided into a set of potential locations (g) for production and storage facilities. Each of these regions is characterized by a given hydrogen demand (\(D_{gt}\)). This set of potential locations along with the associated geographical distribution of the demand must be provided as input data to the problem. The network design can therefore be formally stated as follows.

Given are a fixed time horizon and number of time periods (t), the set of available production (p), storage (s) and transportation technologies (l), the capacity limitations of plants (\(PC_{pl}^{PL}\), \(PC_{pl}^{PL}\)) and storage facilities (\(SC_{s}^{ST}\), \(SC_{s}^{ST}\)) the costs associated with the network operation (facility FOC, and transportation costs TOC), the investment costs (FCC, TCC) the probabilistic information that describe the uncertain parameters (i.e., type of probability distribution, mean and variance) and interest rate (ir).

The final goal is to determine: 1) the optimal SC design, including the number, type, location and capacity of plants and storage facilities (\(N_{gpt}^{PL}, N_{gst}^{ST}\)), along with the number and type of transportation units (\(N_{lt}^{TR}\), e.g. tanker trucks, railway tube cars, etc.), and transportation links to be established between the SC facilities (\(X_{lt}\)); and 2) the associated planning decisions, covering production rates at the plants (\(PR_{igpt}\)), inventory levels at the storage facilities (\(S_{gst}\)) and flows of hydrogen between plants, storage facilities and final markets (\(Q_{igg'lt}\)); in order to minimize simultaneously the total cost and financial risk.
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3. Mathematical Model

The model presented is motivated by previous formulations [3, 4, 5, 6]. Specifically, our approach relies on a multi-period optimization model that extends the formulations previously presented by the authors in order to account for more production and transportation technologies and study the evolution of the network over time. The model also considers the uncertainty of the coefficients of the objective function via a multi-scenario stochastic programming approach.

Particularly, the mathematical formulation considers the possibility of establishing different production, storage and transportation facilities, which are represented by specific integer variables \( N_{PL}^{gpt}, N_{ST}^{gst}, N_{TR}^{lt} \), in a set of potential locations with known demand and uncertain operating costs. The establishment of transportation links between the potential locations is modeled through a binary variable \( X_{gg'lt} \).

The mathematical formulation can be divided into three main blocks of equations, which include the mass balance constraints, the capacity constraints and the objective function equations.

3.1. Mass balance equations

The mass balance must be satisfied in each potential location \( g \) and time period \( t \). Thus, for every hydrogen form \( i \), liquid or gas, the initial inventory kept in a location \( S_{gst}^{-1} \) plus the amount produced \( P_{igpt} \) and the input flow rate \( Q_{ilg'gt} \) must equal the final inventory \( S_{igt} \) plus the amount delivered to the customers \( D_{igt} \) and the output flow rate \( Q_{ilgg't} \):

\[
\sum_{i \in SI(i)} S_{igt-1} + P_{igpt} + \sum_{g \neq g'} \sum_{i} Q_{ilg'gt} = \sum_{i \in SI(i)} S_{igt} + D_{igt} + \sum_{g \neq g'} Q_{ilgg't} \quad \forall i, g, t
\]

In this equation, \( SI(i) \) represents the set of technologies that can be used to store product form \( i \).

3.2. Capacity constraints

Equations 2 and 3 are applied to limit the capacity expansions of production and storage technologies within lower and upper bounds.

\[
NP_{gpt}^{PL} \leq CE_{gpt}^{PL} \leq NP_{gpt}^{PL} \quad \forall g, p, t
\]

\[
NS_{gst}^{ST} \leq SE_{gst}^{ST} \leq NS_{gst}^{ST} \quad \forall g, s, t
\]

Regarding the transportation flows, a zero value of the binary variable \( X_{gg'lt} \) prevents the flow of materials between potential locations from taking place, whereas a value of one allows for the transport of materials within some specified lower and upper bounds.

\[
Q_{i}^{\text{min}} X_{lg'g'e} \leq \sum_{i \in SI(i)} Q_{ilg'g'e} \leq Q_{i}^{\text{max}} X_{lg'g'e} \quad \forall l, g, g', t, e
\]

3.3. Objective function

The expected total cost is given by the mean value of the cost distribution:
\[ E[TDC] = \sum_e \text{prob}_e TDC_e \]

The total cost (TDC) is calculated as the summation of the discounted costs associated with each time period:

\[ TDC_e = \sum_t \frac{TC_{te}}{(1 + ir)^t} \quad \forall e \]

In the aforementioned expressions, \( e \) is the number of scenarios implemented to represent the uncertain parameters space, and \( \text{prob}_e \) is the probability of occurrence associated to each scenario. The equations that model the establishment of gas pipelines and maritime transportation facilities are omitted here due to space limitations. In Equation 6, \( ir \) represents the interest rate and \( TC_{te} \) is the total amount of money spent in period \( t \) and scenario \( e \), which includes the capital (\( FCC_t \), \( TCC_t \)) as well as operating costs (\( FOC_{te} \), \( TOC_{te} \)) given by the production, storage and transportation facilities of the network:

\[ TC_{te} = FCC_t + TCC_t + FOC_{te} + TOC_{te} \quad \forall t,e \]

4. **Financial Risk**

In this work, the probability of meeting unfavorable scenarios is controlled by adding the worst case cost as an additional objective to be minimized. This specific risk metric is easy to implement and leads to good numerical performance in stochastic models [9]. It can be determined from the maximum cost attained over all the scenarios as follows:

\[ WC \geq TDC_e \quad \forall e \]

5. **Solution Strategy: Two-step Sequential Approach**

Our solution method is a two-step sequential approach that exploits the specific structure of the model. Inspired by previous bi-level decomposition methods presented so far in the literature [6, 7], the method relies on decomposing the original formulation into two hierarchical levels: a lower bound master problem (MP) and an upper bound slave problem (SP), that are solved in a sequential way. The master problem corresponds to a specific relaxation of the integer variables of the problem (\( N_{gpt}^M, N_{gst}^M, N_{gl}^{TR} \)), whereas the slave problem is obtained from the original full-space model rounding up some relaxed integer variables provided by the master problem solution.

6. **Results and Discussion**

All the problems were implemented in GAMS [10] and solved in an AMD Phenom™ 8600 B Triple-Core 2300 MHz processor machine using CPLEX 9.0. We first solved several problems that differed in the level of complexity (i.e., number of time periods). The goal is to illustrate the performance of the proposed solution method as compared to the full-space model. The results show that the two-step sequential approach provides near optimal solutions in CPU times that are on average one order of magnitude lower than those reported by the full-space approach. The difference between the lower bound (MP) and the upper bound (SP) remains below 1% for resolutions up to eight periods.
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The model contains 19 potential locations representing the autonomous communities of Spain, whose hydrogen demand is supposed to cover 60% of the actual fossil fuels demand. Hydrogen can be obtained from four different production technologies, each one with the ability of producing liquefied or gaseous hydrogen, two different storage technologies, and six types of transportation modes including road, railway, pipelines and maritime transportation facilities. The length of the time horizon is twelve years and is divided in bi-annual periods. The uncertainty is represented by fifty scenarios, generated using Monte Carlo sampling on a set of normal distributions that characterize the uncertain operating costs. Specifically, in this particular example we aim to analyze the impact that the large variability in the natural gas price has on the SC design.

Figure 1. Pareto curve for slave problem using the 2-step sequential approach.

Figure 1 presents the Pareto frontier of the multi-objective problem. The results obtained show that in order to minimize the worst case, the model resolves to shift from steam methane reforming to coal gasification. This is because the natural gas price shows higher variability than the coal. Let us note that both technologies include carbon sequestration facilities for reducing the GHG emissions.

Figure 2. Cumulative probability curves of the Pareto extreme solutions.
Figure 2 depicts the cumulative probability curves of the feasible extreme of the Pareto set. The figure reveals that for low cost levels (lower than $1.557 \times 10^{12}$ €), the minimum cost solution shows a level of risk lower than the minimum worst case one. The former solution represents a hydrogen network composed by steam methane reforming plants, whereas the latter one involves a mixture of production plants dominated by coal gasification ones. On the other hand, for high cost levels, the coal gasification technology shows less financial risk than steam methane reforming. These extreme solutions and the ones in between reflect different possible attitudes towards.

7. Conclusions
This work has introduced a novel decision-support tool for risk management in the strategic design and planning of hydrogen supply chains under uncertainty in production cost. The problem has been posed as a bi-criteria stochastic MILP that simultaneously accounts for the minimization of the expected cost and the worst case. A new two-step sequential approach has also been presented in order to expedite the solution of such model. Numerical results have shown the convenience of replacing steam methane reforming by coal gasification to reduce the variability of the cost distribution. The approach presented is relevant to guide policy makers towards the adoption of more robust solutions in the face of uncertainty.

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