

# A Bi-Criterion Optimization Approach for the Design and Planning of Hydrogen Supply Chains for Vehicle Use

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*In this article, we address the design of hydrogen supply chains for vehicle use with economic and environmental concerns. Given a set of available technologies to produce, store, and deliver hydrogen, the problem consists of determining the optimal design of the production-distribution network capable of satisfying a predefined hydrogen demand. The design task is formulated as a bi-criterion mixed-integer linear programming (MILP) problem, which simultaneously accounts for the minimization of cost and environmental impact. The environmental impact is measured through the contribution to climate change made by the hydrogen network operation. The emissions considered in the analysis are those associated with the entire life cycle of the process, and are quantified according to the principles of Life Cycle Assessment (LCA). To expedite the search of the Pareto solutions of the problem, we introduce a bi-level algorithm that exploits its specific structure. A case study that addresses the optimal design of the hydrogen infrastructure needed to fulfill the expected hydrogen demand in Great Britain is introduced to illustrate the capabilities of the proposed approach. © 2009 American Institute of Chemical Engineers AIChE J, 56: 650–667, 2010*

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## Introduction

The use of hydrogen as an alternative fuel and energy carrier is receiving increasing interest as the environmental impact of hydrocarbons becomes more evident. Hydrogen

can be produced safely, is environmentally friendly and has many potential energy uses, including powering road vehicles and aircrafts, and heating homes and offices. In particular, its use as a transportation fuel in fuel cell vehicles offers potentially attractive advantages over existing energy sources, particularly regarding emissions of greenhouse gases over the entire life cycle.<sup>1</sup>

Nowadays, most of the hydrogen is produced in petroleum refineries or in the chemical industry, mostly via steam

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reforming. The hydrogen obtained is usually consumed on-site rather than sold on the market, and is mainly used as a feedstock for petroleum refining and for the manufacture of ammonia fertilizer, plastic, resins, solvents, and other industrial commodities. Little hydrogen is currently utilized as an energy source, or as an energy carrier to transport energy from the production to the consumption sites. Specifically, only about 5 % of hydrogen is considered as “marketable” and delivered elsewhere as a liquid or gas by truck or pipeline.<sup>2</sup> Thus, there is still a large gap to achieve the transition from the current fossil-based economy towards a new one based on hydrogen.

The adoption of hydrogen in the current energy system depends to a large extent on the ability to solve the technological problems posed by the aforementioned transition process. In this regard, one of the key issues that still remains open is how to determine the optimal structure of the network capable of fulfilling the growing hydrogen demand in the existing markets. In this context, minimizing exclusively the total cost may lead to solutions that do not fully exploit the environmental benefits of switching to a more sustainable energy system. To avoid this situation, the design task must be posed as a multicriteria decision-making problem, which allows for the simultaneous assessment of environmental and economic concerns at the early stages of the process development.<sup>1</sup> Despite the importance of performing such an analysis, the current situation is that there is a lack of systematic decision-support methods to facilitate this task, mainly because very little research has been conducted to date in this area.

The aim of the present work is to address the environmentally conscious design of hydrogen networks. Specifically, the main objectives of this paper are: (1) to present a bi-criterion formulation that considers simultaneously the total cost and life cycle impact of the hydrogen infrastructure and (2) to develop an efficient solution method that overcomes the numerical difficulties associated with the resulting large-scale MILP.

The article is organized as follows. In first place, a literature review of the topic is presented. A formal definition of the problem under study is next given, along with the bi-criterion MILP used to solve it. The following section introduces a tailor-made decomposition strategy that reduces the computational burden of the model by exploiting its mathematical structure. The capabilities of the proposed modeling framework and solution strategy are next illustrated through a case study based on a real scenario, for which the set of Pareto efficient solutions are calculated. The conclusions of the work are finally drawn in the last part of the article.

## Literature Review

Driven by environmental concerns and energy security, the idea of a “hydrogen economy” has been gaining followers not only in the scientific and engineering areas but also in politics and businesses.<sup>3</sup> Several converging forces explain the interest in hydrogen. First, the technological advances made in different fields such as fuel cells, which are regarded as the potential successors to batteries, power plants, and internal combustion engines. Secondly, the growing competition in the energy industry. Finally, in third place but maybe of greater importance, are the energy-related

problems such as the energy security, air pollution, and climate change, which question the sustainability of the current energy system. In this regard, hydrogen would play a fundamental role in reducing worldwide CO<sub>2</sub> emissions, thus contributing to avoid global warming.

To promote the hydrocarbon economy, government and industry are encouraging the use of gasoline and methanol as sources of hydrogen. A cleaner path based on obtaining hydrogen from natural gas and renewable energy, or using the fuel directly on vehicles, has received much less support, in part because the cost of building a hydrogen infrastructure is widely viewed as prohibitively high. However, several recent studies indicate that the transition towards a hydrogen energy system may be much cleaner and far less expensive than expected.<sup>2</sup>

Iceland was one of the first pioneers in studying the feasibility and advantages of a hydrogen economy, announcing in 1999 its intention to become the world’s first hydrogen society.<sup>4</sup> Hawaii and the South Pacific island of Vanuatu, have also promoted the hydrogen economy, whereas in China, the use of polygeneration using coal as a feedstock may become an economic source of hydrogen.<sup>5,6</sup>

In the private sector, over 100 companies are seeking to commercialize fuel cells for a broad range of applications. Hydrogen is being researched for direct use in automobiles and planes and the most important suppliers of energy and automobile manufacturers are creating divisions of hydrogen and making significant investments in this area.<sup>7</sup>

Unfortunately, despite the potential benefits, and the previous attempts towards a hydrogen economy, its full realization faces a number of social, technical and economic obstacles. Hydrogen still needs to be included into the energy policies and strategies of administration, which tends to preserve the hydrocarbon-based status quo. Furthermore, today’s energy market leads to artificially low fossil fuel prices and encourages the production and use of those fuels, making it difficult for hydrogen and fuel cells to compete with the deep-rooted gasoline-run internal combustion engines and coal-fired power plants.<sup>8</sup> Ogden and her colleagues<sup>9</sup> point out that environmental considerations will be a key issue in the hydrogen transition that is expected to take place in the automotive industry. In this regard, the adoption of strong policies such as zero-emission targets or fiscal incentives will be a critical determinant of the success of fuel cell vehicles.

One of the most significant obstacles to achieve the hydrogen transition is the general perception that a hydrogen supply chain (SC) - the system for producing, storing, and delivering the gas - would be prohibitory expensive to build, in comparison with a system based on gasoline. Thus, automotive and energy companies are investing millions of dollars in the development of reformer and vehicle technologies to obtain and use hydrogen, keeping the current petroleum-based infrastructure unchanged.<sup>10</sup> Along these lines, Jensen and Ross<sup>11</sup> state that the widespread introduction of hydrogen into car fleets faces three main technical challenges. The first is integrating small, inexpensive, and efficient fuel cells into the vehicles. The second is the improvement of storage technologies. Finally, the third and most important one in terms of economic and environmental impact, is developing an efficient infrastructure for producing and delivering hydrogen.

Much of the early work in the area of hydrogen supply chains has been promoted by US legislative pressures, like was done in California in order to improve air quality. In this context, Ogden et al.<sup>9,12</sup> examined different short-term options for producing and delivering compressed gaseous hydrogen through commercially available technologies for production, storage, and distribution. For a longer term, Ogden<sup>13</sup> studied other centralized methods for hydrogen production, including gasification of biomass, coal or municipal solid waste, electrolysis based on wind, solar and nuclear energy.

Furthermore, the design of hydrogen supply chains has also attracted increasing attention in the UK. Guy<sup>14</sup> examined the development of a logistic infrastructure in London and the Southeast, whereas Joffe and coworkers<sup>15</sup> presented a methodology for modeling a hydrogen infrastructure for refueling buses in London and an analysis of the technical issues for installing a hydrogen facility. The authors concluded that the endeavor is both feasible and economically attractive, despite some technical challenges that will be overcome in the near future as technology progresses.

The performance of different pathway options to produce and deliver hydrogen has also been assessed in other comparative studies.<sup>16,17</sup> Although these approaches provide valuable insights into the hydrogen infrastructure, they usually restrict the analysis to a reduced number of options, which represents a major limitation. The alternative to these methods is to develop mathematical programming models capable of generating and assessing in a systematic way a very large number of process alternatives.

In one of the first contributions made in this area, van den Heever and Grossmann<sup>18</sup> discussed the integration of production planning and scheduling for the optimization of a hydrogen supply network. This work addressed the operational level of an existing network but did not take into account design aspects.

Hugo et al.<sup>1</sup> introduced a generic optimization-based model for the optimal design and planning of hydrogen infrastructures. This model utilized formal optimization techniques to assess diverse process alternatives in terms of investment and environmental impact. The model applied an end-of-pipe approach that aimed at reducing the well-to-wheel greenhouse gas emissions.

More recently, Almansoori and Shah<sup>19</sup> presented a mathematical programming approach to design and operate a future British hydrogen supply chain.

Despite the studies and projects devoted to hydrogen, most of them focus on a particular component of the hydrogen supply chain, such as technologies for production, storage or distribution, instead of adopting a systems approach for designing and operating the whole infrastructure as a single entity.<sup>19</sup> These simplifications aim at reducing the complexity of the problem, the size of which grows exponentially as one enlarges the scope of the analysis to include other echelons of the hydrogen supply chain. Moreover, another disadvantage of the aforementioned works is that the joint analysis of the technical feasibility, economic and environmental issues is usually omitted.

With the aim to overcome these limitations, this work presents a holistic approach to address the optimal design of hydrogen supply chains with environmental and economic concerns. Our method relies on the combined use of mathe-

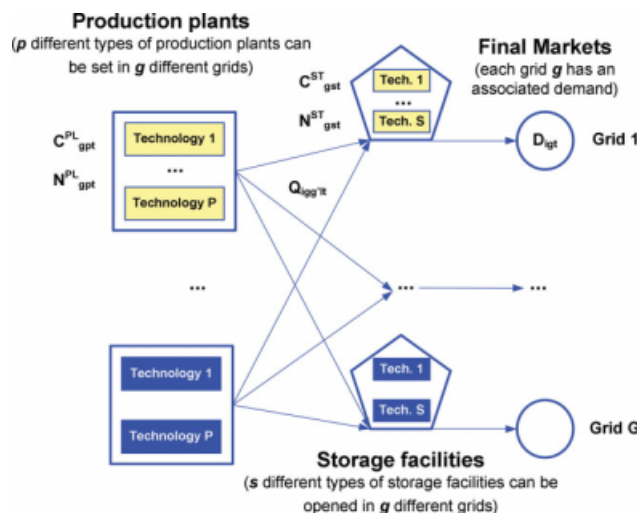


Figure 1. Three-echelon supply chain taken as reference.

[Color figure can be viewed in the online issue, which is available at [www.interscience.wiley.com](http://www.interscience.wiley.com).]

tical programming and LCA principles, which enables the automatic generation and assessment of process alternatives that may lead to significant environmental and economic benefits. The approach presented is complemented with an efficient solution method that makes it possible to address large-scale problems arising in real-world situations.

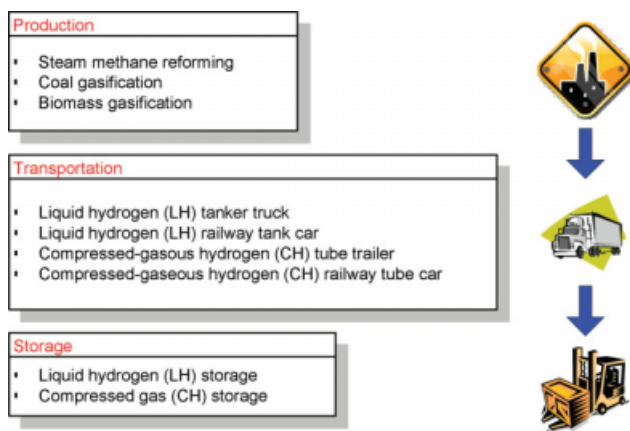
## Problem Statement

We address the optimal design of a typical three-echelon hydrogen SC for vehicle use (see Figure 1). Such a network includes a set of plants where hydrogen is produced, and a set of storage facilities, where hydrogen is stored before being delivered to the final customers. A superstructure of technologies is postulated in which all different alternatives for production, storage and transportation of hydrogen are embedded. Specifically, the superstructure considered in this work is based on the one introduced by Almansoori and Shah,<sup>19</sup> which addressed the design of a SC for vehicle use in UK. Such a superstructure includes the following technological alternatives (see Figure 2):

- Production technology: steam methane reforming, coal gasification and biomass gasification.
- Storage technology: liquid hydrogen storage and compressed gas storage.
- Transportation technology: liquid hydrogen (LH<sub>2</sub>) tanker truck, liquid hydrogen railway tank car, compressed-gaseous hydrogen (CH<sub>2</sub>) tube trailer, compressed-gaseous hydrogen railway tube car.

Note that, in general, the superstructure on which the mathematical formulation is based should be derived according to the specific features of the problem being solved. Examples of other types of superstructures employed in the design of hydrogen SCs can be found elsewhere.<sup>20–22</sup>

The SC entities that implement the technologies embedded in the superstructure can be established in a set of potential locations or grids that are distributed all over the region of interest. Each of these locations has an associated hydrogen demand to be fulfilled either locally or by importing



**Figure 2. Set of alternatives considered in the superstructure.**

[Color figure can be viewed in the online issue, which is available at [www.interscience.wiley.com](http://www.interscience.wiley.com).]

hydrogen from other grids. This set of grids along with the associated geographical distribution of the demand must be provided as input data by the decision-maker. The environmentally conscious network design problem can therefore be stated as follows:

- Given are a fixed time horizon, the demand of hydrogen in each grid and time period, investment costs and capacity limitations of manufacturing and storage facilities, costs associated with the network operation (raw materials, operating, transportation and inventory costs), environmental data (emissions associated with the network operation and damage model) and interest rate.
- The goal is to determine the SC configuration along with the planning decisions that simultaneously minimize the total cost and environmental impact. The major decisions are:
  - Structural decisions: number, types of manufacturing and storage technologies, location and capacity of plants and storage facilities; number and type of transportation units (e.g. tanker trucks, railway tube cars, etc.) and transportation links to be established between the SC entities.
  - Planning decisions for each time period: production rates at the plants; inventory levels at the storage facilities; flows of hydrogen between plants and storage facilities and sales of products.

The mathematical formulation proposed to address this problem is described in the following section.

## Mathematical Model

The model presented is inspired on the work by Almansoori and Shah,<sup>19</sup> in which the authors proposed a steady state “snapshot” formulation of a hydrogen network that considers a time-invariant demand. Specifically, our mathematical formulation modifies and extends the original one in order to account for the evolution of the network over time and a time-variant demand. Furthermore, an additional feature of our model is the inclusion of environmental concerns that are optimized along with the traditional economic objec-

tive. This consideration has led to a bi-criterion decision-making problem, the solution of which comprises a set of Pareto optimal points that trade off cost and environmental impact.

The mathematical formulation presented next is based on the superstructure introduced in the previous section. However, both the superstructure of alternatives as well as the model could be easily modified in order to deal with other additional manufacturing and storage technologies found in a particular industrial scenario. The model presented includes four main sets of equations that are next described in detail.

### Mass balance constraints

The mass balance must be satisfied in every grid and time period. Thus, for every hydrogen form  $i$ , the initial inventory kept in a grid ( $S_{igst-1}$ ) plus the amount produced ( $PR_{igpt}$ ) and the input flow rate ( $Q_{ig'gt}$ ), must equal the final inventory ( $S_{igst}$ ) plus the amount delivered to the customers ( $D_{igst}$ ) and the output flow rate ( $Q_{igg't}$ ).

$$\sum_{s \in SI(i)} S_{igst-1} + \sum_{p \in PI(i)} PR_{igpt} + \sum_{g' \neq g} \sum_l Q_{ig'gt} = \sum_{s \in SI(i)} S_{igst} + D_{igst} + \sum_{g' \neq g} \sum_l Q_{igg't} \quad \forall i, g, t \quad (1)$$

In this equation,  $PI(i)$  denotes the set of manufacturing technologies that can produce hydrogen in form  $i$ , whereas  $SI(i)$  represents the set of storage facilities that can be used to store product in form  $i$ . Furthermore, the total amount of hydrogen in any form  $i$  consumed in grid  $g$  in period  $t$  must be lower than the hydrogen demand in that location ( $\overline{D}_{gt}$ ) and greater than a minimum desired percentage (dsat) of the total demand. This percentage represents the minimum demand satisfaction level that the decision-makers want to achieve:

$$\overline{D}_{gt} \text{dsat} \leq \sum_i D_{igt} \leq \overline{D}_{gt} \quad \forall g, t \quad (2)$$

### Capacity constraints

The mathematical formulation presented here applies simple representations of capacity to model the manufacturing and storage facilities of the network. Such an approximation has been widely applied in SC design problems arising in different industrial scenarios<sup>23</sup> in order to avoid nonlinearities. Specifically, the model includes three main sets of capacity constraints that are applied to the manufacturing plants, storage facilities, and transport links.

**Plants.** The capacity of each plant technology  $p$  that produces product form  $i$  at grid  $g$  in period  $t$  is represented by a continuous variable denoted by  $C_{gpt}^{\text{PL}}$ . Equation 3 constraints the total production rate of technology  $p$  ( $PR_{igpt}$ ) to be lower than the existing capacity and higher than a minimum desired percentage,  $\tau$ , of the available installed capacity:

$$\tau C_{gpt}^{\text{PL}} \leq \sum_{i \in IP(p)} PR_{igpt} \leq C_{gpt}^{\text{PL}} \quad \forall g, p, t \quad (3)$$

In this equation,  $IP(p)$  represents the set of product forms that can be produced via technology  $p$ . The capacity of technology  $p$  at grid  $g$  in any time period  $t$  is calculated from the existing capacity at the end of the previous period plus the expansion in capacity carried out in  $t$  ( $CE_{gpt}^{PL}$ ):

$$C_{gpt}^{PL} = C_{gpt-1}^{PL} + CE_{gpt}^{PL} \quad \forall g, p, t \quad (4)$$

It should be noted that to implement a capacity expansion, there must be a lead time before time  $t$  that is equal to the time of building the corresponding expansion.

Equation 5 is applied to bound the capacity expansions within lower and upper limits. These limits are calculated from the number of plants installed in the grid ( $N_{gpt}^{PL}$ ) and the minimum and maximum capacities associated with each technology  $p$  ( $PC_p^{PL}$  and  $PC_p^{PL}$ , respectively).

$$\underline{PC}_p^{PL} N_{gpt}^{PL} \leq CE_{gpt}^{PL} \leq \overline{PC}_p^{PL} N_{gpt}^{PL} \quad \forall g, p, t \quad (5)$$

**Storage Facilities.** The storage capacity of product form  $i$  during period  $t$  in grid  $g$  associated with technology  $s$  is represented by the continuous variable  $C_{gst}^{ST}$ . Equation 6 forces the total inventory of product in form  $i$  kept at the end of any period  $t$  at the storage facilities of type  $s$  installed in grid  $g$  to be lower than the available capacity.

$$\sum_{i \in IS(s)} S_{igst} \leq C_{gst}^{ST} \quad \forall g, s, t \quad (6)$$

In this equation,  $IS(s)$  denotes the set of product forms  $i$  that can be stored by technology  $s$ . Furthermore, the amount of hydrogen delivered by the storage facilities to the final customers is constrained by their capacity. Thus, this work considers that the capacity required to handle a given amount of hydrogen, assuming regular shipment and delivery schedule, is twice the average storage inventory level kept at the storage facility.<sup>24</sup> During steady-state operation, the average inventory of a product form  $i$  in grid  $g$ , is determined from the amount delivered to customers ( $D_{igt}$ ) and the storage period  $\theta$ . The storage period is introduced to cover fluctuations in both supply and demand as well as plant interruptions:<sup>19</sup>

$$2(\theta D_{igt}) \leq \sum_{s \in SI(i)} C_{gst}^{ST} \quad \forall i, g, t \quad (7)$$

Finally, the capacity of the storage technology at any time period is determined from the previous one and the expansion in capacity executed in the same period ( $CE_{gst}^{ST}$ ):

$$C_{gst}^{ST} = C_{gst-1}^{ST} + CE_{gst}^{ST} \quad \forall g, s, t \quad (8)$$

Similarly, as with the manufacturing plants, the value of  $CE_{gst}^{ST}$  is bounded within lower and upper limits. These bounds are given by the number of storage facilities installed in the grid ( $N_{gst}^{ST}$ ) and the corresponding minimum and maximum storage capacities associated with each storage

technology  $s$  ( $\underline{SC}_s^{ST}$  and  $\overline{SC}_s^{ST}$ , respectively), as stated in Eq. 9:

$$\underline{SC}_s^{ST} N_{gst}^{ST} \leq CE_{gst}^{ST} \leq \overline{SC}_s^{ST} N_{gst}^{ST} \quad \forall g, s, t \quad (9)$$

**Transportation Constraints.** These constraints make use of the binary variable  $X_{gg't}$ , which takes a value of one if a transportation link of type  $l$  (i.e., tanker trucks, railway tube cars, etc.) is established between grids  $g$  and  $g'$  in time period  $t$ , and zero otherwise. The definition of such a variable is enforced via Eq. 10.

$$\underline{QC}_{lgg'} X_{gg't} \leq \sum_{i \in IL(l)} Q_{igg't} \leq \overline{QC}_{lgg'} X_{gg't} \quad \forall g, g' (g \neq g'), l, t \quad (10)$$

Note that a zero value of the aforementioned binary variable prevents the flow of those materials that can be transported via technology  $l$  ( $i \in IL(i)$ ) from taking place, whereas a value of one allows the transport flows within some lower ( $\underline{QC}_{lgg'}$ ) and upper limits ( $\overline{QC}_{lgg'}$ ). Furthermore, a grid can either import or export hydrogen, but not both at the same time. This is because if a grid can only satisfy its needs by importing from other grids, it would not make sense for that grid to export to other grids. This logic condition can be mathematically expressed as follows:

$$X_{gg't} + X_{g'gt} \leq 1 \quad \forall g, g' (g \neq g'), l, t \quad (11)$$

## Objective Function

The mathematical formulation presented before has as an aim to optimize the economic and environmental performance of the hydrogen network. The economic objective is represented by the total discounted cost, whereas the environmental impact is measured through its contribution to climate change.

## Total cost

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

$$TDC = \sum_t \frac{TC_t}{(1+ir)^{t-1}} \quad (12)$$

In this equation,  $ir$  represents the interest rate and  $TC_t$  is the total amount of money spent in period  $t$ , which includes the capital ( $FCC_t$ ,  $TCC_t$ ) as well as operating costs ( $FOC_t$ ,  $TOC_t$ ) given by the production, storage and transportation facilities of the network:

$$TC_t = FCC_t + TCC_t + FOC_t + TOC_t \quad \forall t \quad (13)$$

The calculation of each of these terms is described in detail in the next sections.

**Facility Capital Cost.** The facility capital cost in period  $t$  ( $FCC_t$ ) is determined from the capacity expansions made in

the manufacturing plants and storage facilities during that period as follows:

$$FCC_t = \sum_g \sum_p \left( \alpha_{gpt}^{PL} N_{gpt}^{PL} + \beta_{gpt}^{PL} CE_{gpt}^{PL} \right) + \sum_g \sum_s \left( \alpha_{gst}^{ST} N_{gst}^{ST} + \beta_{gst}^{ST} CE_{gst}^{ST} \right) \quad \forall t \quad (14)$$

The parameters  $\alpha_{gpt}^{PL}$ ,  $\beta_{gpt}^{PL}$  and  $\alpha_{gst}^{ST}$ ,  $\beta_{gst}^{ST}$  appearing in Eq. 14 are the fixed and variable investment terms corresponding to plants and storage facilities, respectively. Note that this equation reflects the concept of economies of scale.

**Transportation Capital Cost.** The transportation capital cost, which includes the cost of the trucks and railcars required to satisfy the demand, is calculated via constraint 15:

$$TCC_t = \sum_l N_{lt}^{TR} \cdot cc_{lt} \quad \forall t \quad (15)$$

Here,  $cc_{lt}$  represents the capital cost associated with transport mode  $l$  in period  $t$ , whereas  $N_{lt}^{TR}$  is an integer variable that denotes the total number of transportation units of type  $l$  purchased in period  $t$  that can transport product  $i$  (i.e.,  $l \in LI(i)$ ). The average number of trucks and/or railcars required to achieve a given flow of materials among the grids of the network is determined from: (1) the flow rates of products between the grids ( $Q_{igg't}$ ), (2) the transportation mode availability ( $av_l$ ), (3) the capacity of a transport container ( $tcap_l$ ), (4) the average distance traveled between the grids ( $distance_{gg'}$ ), (5) the average speed ( $speed_l$ ), and (6) the loading/unloading time ( $lutime_l$ ), as stated in Eq. 16:

$$\sum_{t' \leq t} N_{t'}^{TR} \geq \sum_{i \in LI(l)} \sum_g \sum_{g' \neq g} \frac{Q_{igg't}}{av_l tcap_l} \times \left( \frac{2 distance_{gg'}}{speed_l} + lutime_l \right) \quad \forall l, t \quad (16)$$

Note that the total number of transportation units available in any period  $t$  includes the ones purchased in the same period  $t$  as well as those acquired in previous periods. Hence, the left hand side of the inequality in Eq. 16 represents the summation of the transportation units purchased in all the time periods  $t'$  going from the first one (i.e.,  $t' = 1$ ) to the current period  $t$  (i.e.,  $t' = t$ ). In this equation,  $LI(l)$  denotes the set of product forms  $i$  that can be transported by transport mode  $l$ . For the sake of simplicity, this work assumes that each transportation facility can only operate between two predefined grids. Thus, in constraint 16, the distance between grids  $g$  and  $g'$  ( $distance_{gg'}$ ) is multiplied by two to account for the return journey of the trucks/railcars.

**Facility Operating Cost.** This term is obtained by multiplying the unit production and storage costs ( $upc_{igpt}$  and  $usc_{igst}$ , respectively) by the corresponding production rates and average inventory levels:

$$FOC_t = \sum_i \sum_g \sum_{p \in PI(i)} upc_{igpt} PR_{igpt} + \sum_i \sum_g \sum_{s \in SI(i)} usc_{igst} (\theta D_{igt}) \quad \forall t \quad (17)$$

### Transportation Operating Cost

The total operating cost associated with the transportation tasks carried out in period  $t$  ( $TOC_t$ ) includes the fuel ( $FC_t$ ), labor ( $LC_t$ ), maintenance ( $MC_t$ ) and general costs ( $GC_t$ ) of the transport units:

$$TOC_t = FC_t + LC_t + MC_t + GC_t \quad \forall t \quad (18)$$

The fuel cost is a function of the fuel price ( $fuelp_{lt}$ ) and fuel usage:

$$FC_t = \sum_i \sum_g \sum_{g' \neq g} \sum_{l \in LI(i)} fuelp_{lt} \frac{2 distance_{gg'} Q_{igg't}}{fuelc_l tcap_l} \quad \forall t \quad (19)$$

In Eq. 19, the fractional term represents the fuel usage, and is determined from the total distance traveled in a trip ( $distance_{gg'}$ ), the fuel consumption of transport mode  $l$  ( $fuelc_l$ ) and the number of trips made per period of time ( $\frac{Q_{igg't}}{tcap_l}$ ). Furthermore, as shown in Eq. 20, the labor transportation cost is a function of the driver wage ( $wage_l$ ) and total delivery time (term inside the brackets):

$$LC_t = \sum_i \sum_g \sum_{g' \neq g} \sum_{l \in LI(i)} wage_{lt} \times \left[ \frac{Q_{igg't}}{tcap_l} \left( \frac{2 distance_{gg'}}{speed_l} + lutime_l \right) \right] \quad \forall t \quad (20)$$

The maintenance cost accounts for the general maintenance of the transportation systems and is a function of the cost per unit of distance traveled ( $cud_l$ ) and total distance driven:

$$MC_t = \sum_i \sum_g \sum_{g' \neq g} \sum_{l \in LI(i)} cud_{lt} \left( \frac{2 distance_{gg'} Q_{igg't}}{tcap_l} \right) \quad \forall t \quad (21)$$

Note that in Eqs. 19–21 the distance is also multiplied by two in order to account for the return journeys of the transport units. Finally, the general cost includes the transportation insurance, license and registration, and outstanding finances. It can be determined from the unit general expenses ( $ge_{lt}$ ) and number of transportation units, as follows:

$$GC_t = \sum_l \sum_{t' \leq t} ge_{lt} N_{t'}^{TR} \quad \forall t \quad (22)$$

### Environmental Impact Assessment: Application of LCA Principles

An imperative reason for pressing on the hydrogen alternative is the risk of climate change. Thus, in this work, the environmental performance of the network is measured by its contribution to climate change, which nowadays represents one of the major environmental concerns. Specifically, such a contribution is assessed by following the principles of Life Cycle Assessment (LCA), in a similar way as was done before by the authors (Guillén-Gosálbez and Grossmann,

submitted).<sup>25,26</sup> The two major advantages of this strategy are that: (1) it allows to cover the entire life cycle of the product, process or activity being assessed, and (2) it includes a damage model that links the emissions released and waste generated with the corresponding environmental damage (i.e., contribution to climate change).

More precisely, this work makes use of the Eco-indicator 99 framework, which includes the most recent advances made in LCA. The Eco-indicator 99 allows for the computation of eleven impact categories, which are further aggregated into a single metric (i.e., Eco-indicator 99) that supports objective environmental assessments.

As mentioned before, the goal of this work is to explore the environmental benefits, in terms of overall contribution to climate change, of adopting a hydrogen economy. For this reason, instead of calculating the Eco-indicator 99 itself, we focus our attention on only one of its impact categories: damage to human health caused by climate change. The computation of this metric follows the first three LCA phases: goal and scope definition, inventory analysis, and impact assessment. The remaining phase, LCA interpretation, is addressed by including the impact assessment results into a bi-criterion optimization framework. These phases are described in detail in the next sections.

*Goal and Scope Definition.* In this stage, the system boundaries and the impact categories are identified. In our specific case, the environmental analysis is restricted to the domain of the hydrogen network. Thus, we perform a “cradle-to-gate” analysis that embraces all the logistic activities of the network, starting from the extraction of raw materials and ending with the delivery of hydrogen to customers. With regard to the impact categories, we only evaluate the damage to human health caused by climate change.

*Inventory Analysis.* The second phase of LCA provides the inputs and outputs of materials and energy associated with the process (Life Cycle Inventory), which are required to calculate the environmental impact.

In the context of hydrogen networks, the environmental burdens are caused by the extraction of raw materials, the manufacturing and storage tasks, and the transportation of materials between grids. Mathematically, the inventory of emissions due to the operation of the network can be expressed as a function of some continuous decision variables of the model. Specifically, for each chemical  $b$ , they can be calculated from the production rates at the plants ( $PR_{igpt}$ ), and the transport flows ( $Q_{igg't}$ ), as stated in Eq. 23.

$$LCI_b = \sum_i \sum_g \sum_{p \in PI(i)} \sum_t PR_{igpt} (\omega_{bp}^{PR} + \omega_{bi}^{ST}) + \sum_i \sum_g \sum_{g' \neq g} \sum_{l \in LI(i)} \sum_t Q_{igg't} distance_{gg'} \omega_{bl}^{TR} \quad \forall b \quad (23)$$

The first term of Eq. 23 represents the emissions associated with the manufacturing and storage tasks. The manufacturing tasks include the extraction of raw materials, the generation of the necessary utilities (i.e., steam, electricity, etc.) and the direct emissions from the main processes. The emissions associated with the storage tasks are due to the generation of the energy required for compressing hydrogen. Finally, the second term of Eq. 23 considers the emissions of the transportation tasks.

In Eq. 23,  $\omega_{bp}^{PR}$ ,  $\omega_{bi}^{ST}$ , and  $\omega_{bl}^{TR}$  denote the life cycle inventory entries (i.e., emissions released) associated with chemical  $b$  per reference flow of activity. In the production and storage of hydrogen, the reference flow is one unit of main product produced/stored. In the transportation tasks, the reference flow is one unit of mass transported per one unit of distance.

*Impact Assessment.* In this stage the process data are translated into environmental information. As was mentioned before, we only consider the damage to human health caused by climate change. The units of this metric are Disability Adjusted Life Years (DALYs). A damage of one means that one life year of one individual is lost, or one person suffers four years from a disability with a weigh of 0.25.

Mathematically, the damage caused is calculated from the life cycle inventory and the corresponding damage factor ( $v_b$ ), as stated in Eq. 24.

$$DAM = \sum_b v_b LCI_b \quad (24)$$

The damage factor represents the link between the results of the inventory phase and the damage in the corresponding impact category. For the human health damage category, the damage model includes: (1) a fate analysis, to link any emission, which is expressed in terms of mass, to a temporary change in concentration, (2) an exposure analysis, to link this temporary concentration to a dose, (3) an effect analysis, to link the dose to a number of health effects, and (4) a damage analysis to translate the health effects into Disability Adjusted Life Years (DALYs).

*Interpretation.* Finally, in the fourth phase the results are analyzed and a set of conclusions or recommendations for the system are formulated. In this regard, the final goal of LCA is to provide criteria and quantitative measures for comparing different process operation and design alternatives. One of the main shortcomings of LCA is that it lacks a systematic way of generating such alternatives and identify the best ones in terms of environmental performance. To circumvent these limitations, in this article we follow a combined approach that consists of coupling LCA and optimization tools within a single decision-making framework.<sup>26–28</sup> Thus, in our work the preferences are articulated in the post-optimal analysis of the Pareto optimal solutions. This approach provides further insights into the design problem and allows for a better understanding of the inherent trade-off between economic and environmental criteria.

#### Other constraints: Bounds on integer variables

The total number of production plants, storage facilities and transportation units can be constrained to be lower than certain upper limits ( $UB_{gp}^{PL}$ ,  $UB_{gst}^{ST}$  and  $UB_{lt}^{TR}$ , respectively). This can be easily done by adding constraints 25–27:

$$N_{gpt}^{PL} \leq UB_{gpt}^{PL} \quad \forall g, p, t \quad (25)$$

$$N_{gst}^{ST} \leq UB_{gst}^{ST} \quad \forall g, s, t \quad (26)$$

$$N_{lt}^{TR} \leq UB_{lt}^{TR} \quad \forall l, t \quad (27)$$

## Solution Strategy

The overall bi-criterion MILP can be expressed as follows:

$$\begin{aligned} \min_{x, X, N} \quad & (\text{TDC}(x, X, N), \text{DAM}(x, X, N)) \\ \text{s.t.} \quad & \text{constraints 1 - 27} \\ & x \in \mathbb{R}, X \in \{0, 1\}, N \in \mathbb{N} \end{aligned}$$

Here,  $x$  denotes the continuous variables of the problem (capacity expansions, production rates, inventory levels and materials flows),  $X$  represents the binary variables (i.e., establishment of transportation links), and  $N$  are the integer variables denoting the number of plants, storage facilities and transportation units of each type selected.

The solution of the bi-criterion MILP introduced before is given by a set of Pareto optimal alternatives that trade off the economic and environmental concerns considered in the analysis. There are two main methods that deal with this type of problems: the weighted-sum method and the  $\varepsilon$ -constraint method.<sup>29</sup> The weighted-sum method, is only rigorous for problems whose Pareto set is convex. On the other hand, the  $\varepsilon$ -constraint method is also rigorous for the nonconvex case, which turned out to be our case. The identification of the trade-off solutions can also be formulated as a parametric programming problem,<sup>30</sup> and solved with tailor made solution algorithms<sup>26</sup> for parametric programming. This last approach is not well suited to multi-objective problems whose Pareto set comprises a high number of different structural solutions (i.e., solutions that differ in the values of the integer variables), like the one addressed in this work.

Hence, in the approach presented, the Pareto solutions of the problem are computed via the  $\varepsilon$ -constraint method, which entails solving a set of instances of model (M) corresponding to different values of the auxiliary parameter  $\varepsilon$ :

$$\begin{aligned} \text{(M)} \quad \min_{x, X, N} \quad & (\text{TDC}(x, X, N)) \\ \text{s.t.} \quad & \text{constraints 1 - 27} \\ & \text{DAM}(x, X, N) \leq \varepsilon \\ & \underline{\varepsilon} \leq \varepsilon \leq \bar{\varepsilon} \\ & x \in \mathbb{R}, X \in \{0, 1\}, N \in \mathbb{N} \end{aligned}$$

where the lower and upper limits within which the epsilon parameter must fall (i.e.,  $\varepsilon \in [\underline{\varepsilon}, \bar{\varepsilon}]$ ) are obtained from the optimization of each separate scalar objective:

$$\begin{aligned} \text{(M1a)} \quad (\bar{x}, \bar{X}, \bar{N}) = \arg \min_{x, X, N} \quad & (\text{DAM}(x, X, N)) \\ \text{s.t.} \quad & \text{constraints 1 - 27} \\ & x \in \mathbb{R}, X \in \{0, 1\}, N \in \mathbb{N} \end{aligned}$$

which defines  $\underline{\varepsilon} = \text{DAM}(\bar{x}, \bar{X}, \bar{N})$  and

$$\begin{aligned} \text{(M1b)} \quad (\bar{x}, \bar{X}, \bar{N}) = \arg \min_{x, X, N} \quad & (\text{TDC}(x, X, N)) \\ \text{s.t.} \quad & \text{constraints 1 - 27} \\ & x \in \mathbb{R}, X \in \{0, 1\}, N \in \mathbb{N} \end{aligned}$$

which defines  $\bar{\varepsilon} = \text{DAM}(\bar{x}, \bar{X}, \bar{N})$ .

To expedite the calculation of the Pareto solutions, we next present a bi-level algorithm that exploits the specific structure of the problem. Our solution procedure relies on

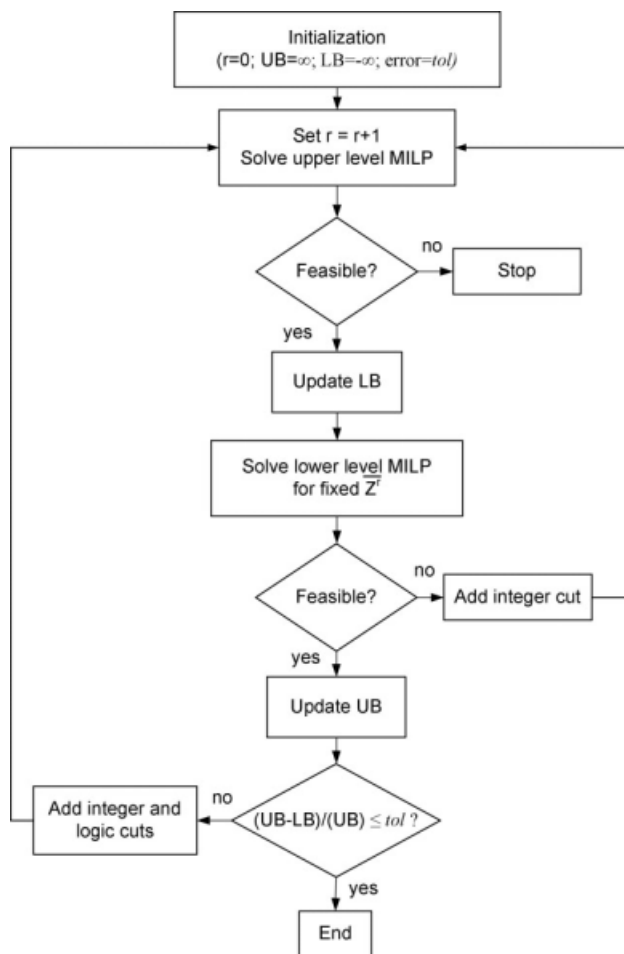


Figure 3. Flowchart for the bilevel decomposition algorithm.

hierarchically decomposing the monolithic formulation (M) into two levels, an upper level master problem (UP) and a lower level slave problem (LO), between which the algorithm iterates until a termination criterion is satisfied.<sup>31</sup>

## Bi-Level Algorithm

The proposed decomposition algorithm (see Figure 3) solves an upper level master problem (UP), which is a specific relaxation of problem (M), to obtain a lower bound on the cost. In the master problem, the integer variables that represent the production plants and storage facilities are removed, whereas the ones associated with the transportation units are relaxed. Furthermore, the master problem includes a set of auxiliary binary variables that are added to represent the selection of a specific technology over the entire planning horizon. Because of these modifications, problem (UP) is combinatorially less complex than the original model (M). The master level of the algorithm provides as output the subset of manufacturing, storage and transport technologies that should be used in the hydrogen infrastructure.

The lower level planning problem (LO) is solved for the selected set of technologies, yielding an upper bound on the total cost of the network for any feasible solution of (UP). As only a subset of processes is selected in (UP), model



(LO) contains fewer integer variables and is not as combinatorially complex as problem (M).

We note that for both problems (UP) and (LO), the equations for all time periods are included for all the processes that are considered. The computational expense is lowered by reducing the number of integer variables in each level. The problems are solved iteratively by adding integer and logic cuts until the bounds converge.

### Upper level problem

The upper level master problem (UP) is obtained from model (M) as follows. The integer variables  $N_{gpt}^{PL}$ ,  $N_{gst}^{ST}$  are removed, whereas variable  $N_{lt}^{TR}$  is relaxed into the continuous variable  $RN_{lt}^{TR}$ . Equations 5 and 9, which impose capacity limitations based on the number of installed facilities, are also removed. Constraint 14 is reformulated as follows:

$$FCC_t = \sum_g \sum_p \left( \alpha_{gpt}^{PL} \frac{CE_{gpt}^{PL}}{PC_p^{PL}} + \beta_{gpt}^{PL} CE_{gpt}^{PL} \right) + \sum_g \sum_s \left( \alpha_{gst}^{ST} \frac{CE_{gst}^{ST}}{SC_s^{ST}} + \beta_{gst}^{ST} CE_{gst}^{ST} \right) \quad \forall t \quad (28)$$

Finally, three new sets of binary variables are added to the model:  $Z_{gp}^{PL}$ ,  $Z_{gs}^{ST}$  and  $Z_l^{TR}$ . These binary variables take a value of one if the corresponding technology, either manufacturing process  $p$ , storage facility  $s$  or transportation mode  $l$ , are selected in grid  $g$ , and zero otherwise. The definition of these variables is enforced via the following constraints:

$$\frac{CE_{gpt}^{PL}}{PC_p^{PL}} \leq Z_{gp}^{PL} UB_{gpt}^{PL} \quad \forall g, p, t \quad (29)$$

$$\frac{CE_{gst}^{ST}}{SC_s^{ST}} \leq Z_{gs}^{ST} UB_{gst}^{ST} \quad \forall g, s, t \quad (30)$$

$$RN_{lt}^{TR} \leq Z_l^{TR} UB_{lt}^{TR} \quad \forall l, t \quad (31)$$

As can be observed, if a technology is not selected (i.e.,  $Z$  equals zero), the associated production rates, inventory levels and transportation units are forced to zero. On the other hand, when the binary variables take a value of one, the technologies are allowed to operate within specific upper bounds ( $UB_{gpt}^{PL}$ ,  $UB_{gst}^{ST}$  and  $UB_{lt}^{TR}$ , respectively). Note that these bounds, which were also used in Eqs. 25–27, represent the maximum number of production plants, storage facilities and transportation units that can be selected.

The upper level problem can therefore be expressed as follows:

$$(UP) \quad \min_{x, X, RN, Z} \quad (TDC(x, X, RN, Z))$$

s.t. constraints 1 – 4, 6 – 8, 10 – 31  
 $DAM(x, X, N) \leq \varepsilon$   
 $\underline{\varepsilon} \leq \varepsilon \leq \bar{\varepsilon}$   
 $x, RN \in \mathbb{R}, X, Z \in \{0, 1\}$

where  $Z$  denotes the new set of auxiliary binary variables. Note that problem (UP) has  $|g|^2 \cdot |l| \cdot |t| + |g| \cdot |p| + |g| \cdot |s| + |l|$

binary variables, whereas problem (M) has  $|g|^2 \cdot |l| \cdot |t|$  binary variables and  $|l| \cdot (|g| \cdot |p| + |g| \cdot |s| + |l|)$  integer variables. Thus, (UP) is combinatorially less complex than (M).

Furthermore, since model (UP) is a relaxation of problem (M), it satisfies the following mathematical property (see the proof in the Appendix):

**Property 1.** *Problem (UP) provides a lower bound to the solution of problem (M).*

### Lower level problem

The lower level is represented by the original MILP model (M), which is solved for only a subset of technologies (i.e., manufacturing plants, storage and transport facilities) predicted at the upper level. The main motivation for this procedure is that the number of integer variables, and, hence, the size of the lower level formulation, is reduced by excluding the technologies that were not selected by the upper level problem through the auxiliary binary variables  $Z$  obtained at iteration  $r$ . This is accomplished by adding the following inequalities:

$$N_{gpt}^{PL} \leq \overline{Z}_{gp}^{PL} UB_{gpt}^{PL} \quad \forall g, p, t \quad (32)$$

$$N_{gst}^{ST} \leq \overline{Z}_{gs}^{ST} UB_{gst}^{ST} \quad \forall g, s, t \quad (33)$$

$$N_{lt}^{TR} \leq \overline{Z}_l^{TR} UB_{lt}^{TR} \quad \forall l, t \quad (34)$$

where  $\overline{Z}_{gp}^{PL}$ ,  $\overline{Z}_{gs}^{ST}$  and  $\overline{Z}_l^{TR}$  denote the optimal values of the auxiliary binary variables of the master problem. Note that constraints 32–34 force the integer variables of (M) to take a zero value if the corresponding auxiliary binary variables are zero, and are equivalent to Eqs. 25–27 otherwise.

The lower level problem can therefore be formally stated as follows:

$$(LO) \quad \min_{x, X, N} \quad TDC(x, X, N)$$

s.t. constraints 1 – 27, 32 – 34  
 $DAM(x, X, N) \leq \varepsilon$   
 $\underline{\varepsilon} \leq \varepsilon \leq \bar{\varepsilon}$   
 $x \in \mathbb{R}, X \in \{0, 1\}, N \in \mathbb{N}$

As can be observed, model (LO) is simply defined by adding to problem (M) the inequalities 32–34. Note that model (LO) yields a valid upper bound to (M), because its search space is contained in the search space of (M). Thus, any feasible solution of (LO) is also a feasible solution of (M). In our algorithm, the upper-level (UP) and the lower-level (LO) problems are solved iteratively until the bounds of each level converge within a specified tolerance.

### Integer and logic cuts

The upper level problem must be resolved at each iteration in order to provide new solutions for the lower level. This procedure is repeated until the termination criterion is satisfied. To expedite the calculation of the master problem, we make use of integer and logic cuts. The integer cuts are employed to exclude the set of solutions explored by the

algorithm in previous iterations. These cuts are mathematically expressed as follows:<sup>32</sup>

$$\sum_{m \in W_1^r} Z_m - \sum_{m \in W_0^r} Z_m \leq |W_1^r| - 1 \quad \forall r \quad (35)$$

where  $W_1^r = \{m | \bar{Z}_m^r = 1\}$  and  $W_0^r = \{m | \bar{Z}_m^r = 0\}$ , with  $\bar{Z}_m^r$  being the value of the  $m$  component of the vector of binary variables in the optimal solution computed in iteration  $r$ . Note that  $W_1^r$  and  $W_0^r$  are both obtained from the optimal solution of the upper level problem in iteration  $r$ .

Furthermore, to reduce the search space and the number of iterations in the decomposition procedure, we employ logic cuts that allow to eliminate suboptimal alternatives. More precisely, we make use of subset cuts, which are motivated by the cuts proposed by Iyer and Grossmann.<sup>31</sup> The following property establishes the basis for the derivation of such cuts (the associated proof can be found in the Appendix):

**Property 2.** Let  $W_1^r = \{m | \bar{Z}_m^r = 1\}$  and  $W_0^r = \{m | \bar{Z}_m^r = 0\}$  correspond to the optimal solution of (UP) in iteration  $r$ . For all iterations  $s > r$ , if  $W_1^r$  is feasible in (LO), then any solution  $W_1^s \subset W_1^r$  will result in a solution of (LO) such that  $TDC_{LO}^s \geq TDC_{LO}^r$ . See appendix for proof.

The cut for precluding subsets can be logically written as:

$$\left( \bigvee_{m \in W_0^r} Z_m \right) \vee Z_n \quad \forall r \quad \forall n \in W_1^r \quad (36)$$

This logic expression can be mathematically translated into the following constraint:

$$\sum_{m \in W_0^r} Z_m + Z_n \geq 1 \quad \forall r \quad \forall n \in W_1^r \quad (37)$$

A description on how to derive cuts from logical inference clauses is given by Raman and Grossmann.<sup>33</sup>

### Algorithmic Steps

The detailed steps of the proposed decomposition strategy, which are applied for every selected value of  $\varepsilon$ , are as follows:

1. Set iteration count  $r = 0$ , upper bound  $UB = \infty$ , lower bound  $LB = -\infty$ , and tolerance error =  $tol$ .
2. Set  $r = r + 1$ . Solve the MILP master problem (UP):
  - If problem (UP) is infeasible, then stop.
  - Otherwise, set the current lower bound to:  $LB = LB^r$ , and define:

$$W_1^r = \{m | \bar{Z}_m^r = 1\} \quad (38)$$

$$W_0^r = \{m | \bar{Z}_m^r = 0\} \quad (39)$$

where  $LB^r$  is the objective function value associated with the optimal solution of (UP) in iteration  $r$ , and  $\bar{Z}^r$  represents the vector of binary variables for the same solution.

3. For fixed  $\bar{Z}^r$ , solve the lower level problem (LO) to obtain a capacity expansion plan and an upper bound to the cost.
  - If problem (LO) is infeasible, then add the following integer cut to (UP) and go to step 2:

$$\sum_{m \in W_1^r} Z_m - \sum_{m \in W_0^r} Z_m \leq |W_1^r| - 1 \quad (40)$$

- Otherwise, update the current upper bound as follows:  $UB = \min\{UB^r\}$ , where  $UB^r$  represents the objective function value associated with the optimal solution of (LO) in iteration  $r$ .
4. Check the convergence criteria:
    - If  $\frac{UB-LB}{UB} \leq tol$ , then stop. The solution corresponding to  $UB$  (i.e., the solution of model (LO) in the iteration with minimum cost) satisfies the termination criterion (i.e., it can be regarded as optimal within the predefined optimality gap).
    - Otherwise, define the set of integer and logic cuts that will be added to problem (UP) in the next iteration:

$$\sum_{m \in W_1^r} Z_m - \sum_{m \in W_0^r} Z_m \leq |W_1^r| - 1 \quad (41)$$

$$\sum_{m \in W_0^r} Z_m + Z_n \geq 1 \quad \forall n \in W_1^r \quad (42)$$

and go to step 2.

### Remarks

- The proposed decomposition algorithm provides the global optimal solution to the original MILP model in a finite number of iterations, since the number of possible production, storage and transport technologies is finite.
- The integer and logic cuts in Eqs. 41 and 42 are added cumulatively at each iteration to the upper-level model (UP), which leads to an increase in its size.
- The master problem can be tightened by adding the following constraints:

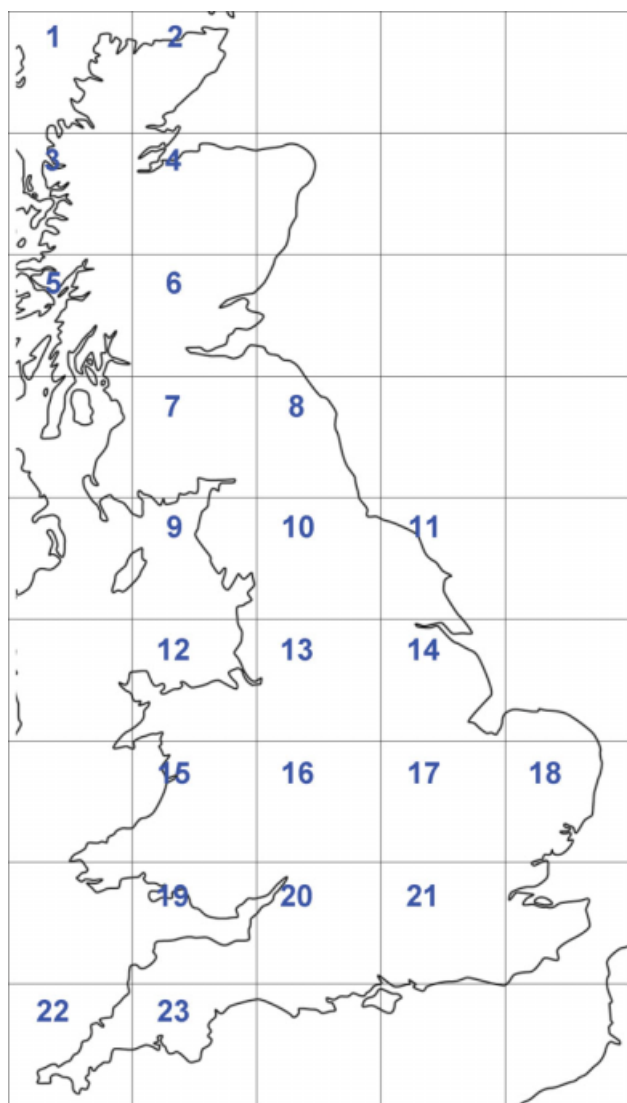
$$\tau_{PC_p}^{PL} Z_{gp}^{PL} \leq \sum_{i \in IP(p)} \sum_t PR_{igpt} \quad \forall g, p \quad (43)$$

$$Z_{gs}^{ST} \leq \sum_t \frac{CE_{gst}^{ST}}{SC_s^{ST}} \quad \forall g, s \quad (44)$$

$$Z_l^{TR} \leq \sum_t RN_{lt} \quad \forall l \quad (45)$$

These equations impose lower limits on the production rates, expansions in the capacity of the storage facilities and number of transportation units if the corresponding processes are selected, and are inactive otherwise. The use of such inequalities leads to tighter bounds, which in turn reduces the computational burden of the algorithm.

- The complexity of our mathematical formulation is mainly given by the number of time periods, regional grids and technological alternatives embedded in the superstructure. In general, the problem size can be decreased by reducing the number of periods and/or grids. This can be done,



**Figure 4. Set of grids (potential locations) for the SC entities in the case study.**

[Color figure can be viewed in the online issue, which is available at [www.interscience.wiley.com](http://www.interscience.wiley.com).]

for instance, by merging different grids and/or time periods into a single grid/period with an aggregated demand that is the summation of the individual ones. If these modifications are not enough to reduce the computational burden of the model and hence to achieve a fast convergence between the lower and upper bounds, there is still the option of setting a nonzero optimality tolerance  $tol$  in step 1 (e.g., 1–5%). Note that even in those cases in which it is difficult to close the gap between the bounds, the proposed procedure might be able to generate good feasible solutions whose global optimality can be guaranteed within the difference of the bounds.

### Case Study

The case study proposed by Almansoori and Shah<sup>19</sup> is used to illustrate the capabilities of our modeling framework and solution strategy. A detailed description of the design problem to be solved can be found in the original work.

**Table 1. Demand for  $t=1$  (Assume an Annual Increase of 5 %)**

Grid	Hydrogen Demand (ton/yr)
1	510
2	400
3	790
4	1195
5	650
6	900
7	2005
8	1925
9	3220
10	4510
11	715
12	2565
13	4985
14	2485
15	3435
16	5235
17	4305
18	1985
19	2285
20	5320
21	15,255
22	1040
23	1260

Some minor details of the case study that must be considered when performing the calculations are commented next for the sake of completeness of our work.

A preprocessing step of the original data provided by the authors was performed in order to decrease the model size. This was accomplished by merging adjacent regions with low demands into aggregated grids. The new grids along with the associated demand are shown in Figure 4 and Table 1. The upper bounds on the number of plants, storage facilities and transportation units considered in the analysis were 20, 250 and 50, respectively. Furthermore, zero upper bounds were imposed on the total number of plants opened in grids 1 and 22 (i.e., we assumed that it is not possible to establish manufacturing facilities in such regions). The fixed and variable investment terms associated with the production and storage facilities, which are given in Tables 2 and 3, were calculated from the investment costs corresponding to the facilities with minimum and maximum capacity. Specifically, the cost of the facility with maximum capacity can be found in the work of Almansoori and Shah,<sup>19</sup> whereas that corresponding to the minimum capacity alternative can be estimated from the former one via the six-tenth rule. The interest rate, the minimum demand satisfaction level and the minimum desired percentage,  $\tau$ , of the available installed capacity were set to 10%, 90%, and 25%, respectively. It was also assumed that raw materials are available at the same price in all the grids.

**Table 2. Fixed and Variable Capital Investment Terms for Plants for  $t=1$  (Assume an Annual Increase of 5 %)**

	$\alpha_{spt}^{PL}$ (\$)		$\beta_{spt}^{PL}$ (\$/kg)	
	LH <sub>2</sub>	CH <sub>2</sub>	LH <sub>2</sub>	CH <sub>2</sub>
Steam reforming	$4.22 \times 10^7$	$2.99 \times 10^7$	2.81	1.99
Coal gasification	$7.55 \times 10^7$	$6.08 \times 10^7$	5.04	4.05
Biomass gasification	$1.11 \times 10^8$	$7.15 \times 10^7$	7.42	4.77

**Table 3. Fixed and Variable Capital Investment Terms for Storage Facilities for  $t=1$  (Assume an Annual Increase of 5 %)**

	$\alpha_{gst}^{ST}$ (\$)	$\beta_{gst}^{ST}$ (\$/kg)
Cryogenic spherical tank (LH <sub>2</sub> )	$9.05 \times 10^6$	209.17
Pressurized cylindrical vessel (CH <sub>2</sub> )	$1.40 \times 10^8$	3247.25

The data of the emission inventories associated with the operation of the hydrogen network (i.e., extraction of raw materials, production, storage and transportation of hydrogen) were estimated from different sources in the literature.<sup>3,34–36</sup> This information was complemented with the Ecoinvent database,<sup>37</sup> from which the emissions associated with the energy generation and transportation tasks were retrieved. Table 4 summarizes the main results of the LCA analysis carried out to determine the environmental impact of the production, storage and transportation tasks. In our study, the parameters of the damage model that translates the emissions released into the damage to human health caused by climate change were taken from the Eco-indicator 99 methodology,<sup>38</sup> assuming the average weighting set and the Hierarchist perspective.

### Computational performance

We first solved several problems of different levels of complexity based on the number of time periods, each of which has a length of one year. The goal is to illustrate the performance of the algorithm as compared to the full-space method. The objective in these problems was to minimize cost as a single objective function.

**Table 4. Environmental Impact Data**

Technology	Impact Due to Climate Change
Steam reforming (DALYs kg <sup>-1</sup> )	$3.34 \times 10^{-6}$
Coal gasification (DALYs kg <sup>-1</sup> )	$6.07 \times 10^{-5}$
Biomass gasification (DALYs kg <sup>-1</sup> )	$-2.58 \times 10^{-5}$
Cryogenic spherical tank (LH <sub>2</sub> ) (DALYs kg <sup>-1</sup> )	$1.44 \times 10^{-7}$
Pressurized cylindrical vessel (CH <sub>2</sub> ) (DALYs kg <sup>-1</sup> )	$3.20 \times 10^{-8}$
Tanker truck (LH <sub>2</sub> ) (DALYs ton <sup>-1</sup> km <sup>-1</sup> )	$3.49 \times 10^{-8}$
Tube trailer (CH <sub>2</sub> ) (DALYs ton <sup>-1</sup> km <sup>-1</sup> )	$7.77 \times 10^{-8}$
Railway tank car (LH <sub>2</sub> ) (DALYs ton <sup>-1</sup> km <sup>-1</sup> )	$7.85 \times 10^{-9}$
Railway tube car (CH <sub>2</sub> ) (DALYs ton <sup>-1</sup> km <sup>-1</sup> )	$1.20 \times 10^{-8}$

All the problems were implemented in GAMS<sup>39</sup> and solved in the full-space using the CPLEX 9.0 solver on an Intel 1.2 GHz machine. Tables 5 and 6 shows the problem sizes and solution times for the proposed decomposition algorithm and the full-space method, both solved for a 1% optimality tolerance. Note that in the case of the decomposition strategy, this gap represents the difference between the solutions of the higher level and lower level problems, and not the optimality gap with which the sub-problems were solved. In all the cases, the termination criterion (i.e., optimality gap) was satisfied in one single iteration.

As can be observed, the proposed approach shows better numerical performance than the full-space method. For small problems ( $t \leq 2$ ), the full-space method is almost as efficient as the decomposition strategy, since the number of integer variables is very small. On the other hand, as the size of the problem increases the differences in CPU time are more significant. Specifically, for  $t \geq 3$ , the decomposition strategy

**Table 5. Computational Results for  $t \leq 5$**

	Variables*			Equations*	Time (s)	Cost (\$)†
	Binary	Discrete	Continuous			
$t=1$						
Full space	2116	188	2545	7103	0.23	$7.5308 \times 10^{10}$
Bilevel					0.29	$7.5308 \times 10^{10}$
LB	2308	–	2545	7111		
UB	2116	45	2545	7103		
$t=2$						
Full space	4232	376	5084	14,200	1.55	$8.5393 \times 10^{10}$
Bilevel					0.77	$8.5314 \times 10^{10}$
LB	4424	–	5088	14,166		
UB	4232	90	5084	14,200		
$t=3$						
Full space	6348	564	7623	21,297	29.36	$9.5180 \times 10^{10}$
Bilevel					11.34	$9.5073 \times 10^{10}$
LB	6540	–	7631	21,221		
UB	6348	135	7623	21,297		
$t=4$						
Full space	8464	752	10,162	28,394	191.75	$1.0493 \times 10^{11}$
Bilevel					21.54	$1.0507 \times 10^{11}$
LB	8656	–	10,174	28,276		
UB	8464	180	10,162	28,394		
$t=5$						
Full space	10,580	940	12,701	35,491	255.97	$1.1492 \times 10^{11}$
Bilevel					44.16	$1.1468 \times 10^{11}$
LB	10,772	–	12,717	35,331		
UB	10,580	225	12,701	35,491		

\*Variables and equations in the first iteration.

†Objective function value with 1% optimality gap.

**Table 6. Computational Results for  $t \geq 6$**

	Variables*			Equations*	Time (s)	Cost (\$)†
	Binary	Discrete	Continuous			
$t=6$						
Full space	12,696	1128	15,240	42,588	523.32	$1.24137 \times 10^{11}$
Bilevel					44.39	$1.24227 \times 10^{11}$
LB	12,888	–	15,260	42,386		
UB	12,696	270	16,098	42,588		
$t=7$						
Full space	14,812	1316	17,779	49,685	1558.95	$1.34135 \times 10^{11}$
Bilevel					55.22	$1.33602 \times 10^{11}$
LB	15,004	–	17,803	49,441		
UB	14,812	315	18,780	49,685		
$t=8$						
Full space	16,928	1504	20,318	56,782	795.90	$1.42362 \times 10^{11}$
Bilevel					180.84	$1.42449 \times 10^{11}$
LB	17,120	–	20,346	56,496		
UB	16,928	360	21,462	56,782		
$t=9$						
Full space	19,044	1692	22,857	63,879	1239.45	$1.51041 \times 10^{11}$
Bilevel					185.33	$1.51059 \times 10^{11}$
LB	19,236	–	22,889	63,551		
UB	19,044	405	24,144	63,879		
$t=10$						
Full space	21,160	1880	25,396	70,976	7195.72	$1.59968 \times 10^{11}$
Bilevel					443.42	$1.59467 \times 10^{11}$
LB	21,352	–	25,432	70,606		
UB	21,160	450	26,826	70,976		

\*Variables and equations in the first iteration.

†Objective function value with 1% optimality gap.

provides near optimal solutions (i.e., with an optimality gap of 1%) in CPU times that are approximately one order of magnitude lower than those reported by the full-space approach. As can be observed, the higher level problem can be solved very quickly, whereas the lower level problem is the bottleneck of the proposed method. Note that in the latter formulation the number of integer variables is significantly decreased in comparison with the full space model. This greatly reduces the combinatorial complexity of the problem, and, thus, its computational burden.

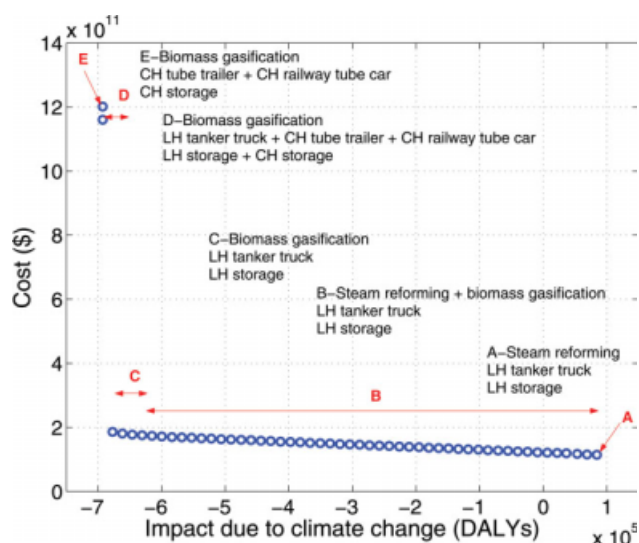
### Pareto solutions and discussion

Having proved the application and computational effectiveness of the proposed algorithm, our approach was next used to generate the complete Pareto set associated with one of the previous examples. Specifically, we solved the problem considering 5 periods (i.e., with a total time horizon of 5 years), and assuming the same data as before.

The values of  $\underline{\varepsilon}$  and  $\bar{\varepsilon}$  that define the search interval for DAM were firstly calculated by maximizing both objectives separately. The original interval  $[\underline{\varepsilon}, \bar{\varepsilon}]$  was next partitioned into 50 subintervals of equal length, and model (M) was then calculated for every possible value of  $\varepsilon$ . The proposed algorithm was solved with an optimality gap (i.e., tolerance) of 1%. The problem size is given in Table 5 (case with 5 periods). The total CPU time required to generate the Pareto solutions was 6,857 CPU seconds.

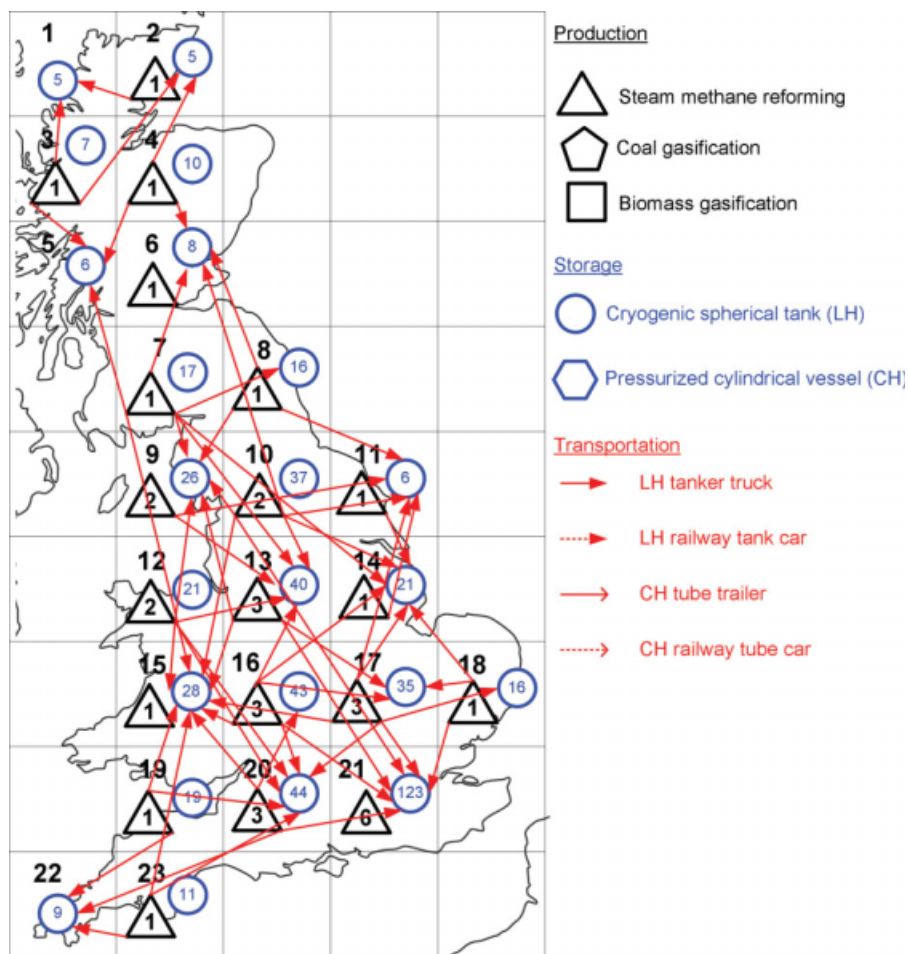
Figure 5 shows the Pareto solutions obtained by following the proposed procedure. Each point of the Pareto set entails a specific SC structure and a set of planning decisions. Note that a natural trade-off exists between total cost and environmental impact, since a reduction in the latter metric can only

be achieved by compromising the cost of the network. Specifically, five different structural alternatives (A,B,C,D and E) were identified in the Pareto set. In the first design A (i.e., minimum cost solution), hydrogen is produced via steam reforming and it is transported and stored as a liquid. In the alternative B, hydrogen is generated from steam as well as biomass gasification, and it is also handled as a liquid. Finally, in designs C,D and E, hydrogen is produced exclusively from biomass. These last alternatives differ in the technology employed to transport and store hydrogen. In



**Figure 5. Pareto set.**

[Color figure can be viewed in the online issue, which is available at [www.interscience.wiley.com](http://www.interscience.wiley.com).]



**Figure 6. Minimum cost solution.**

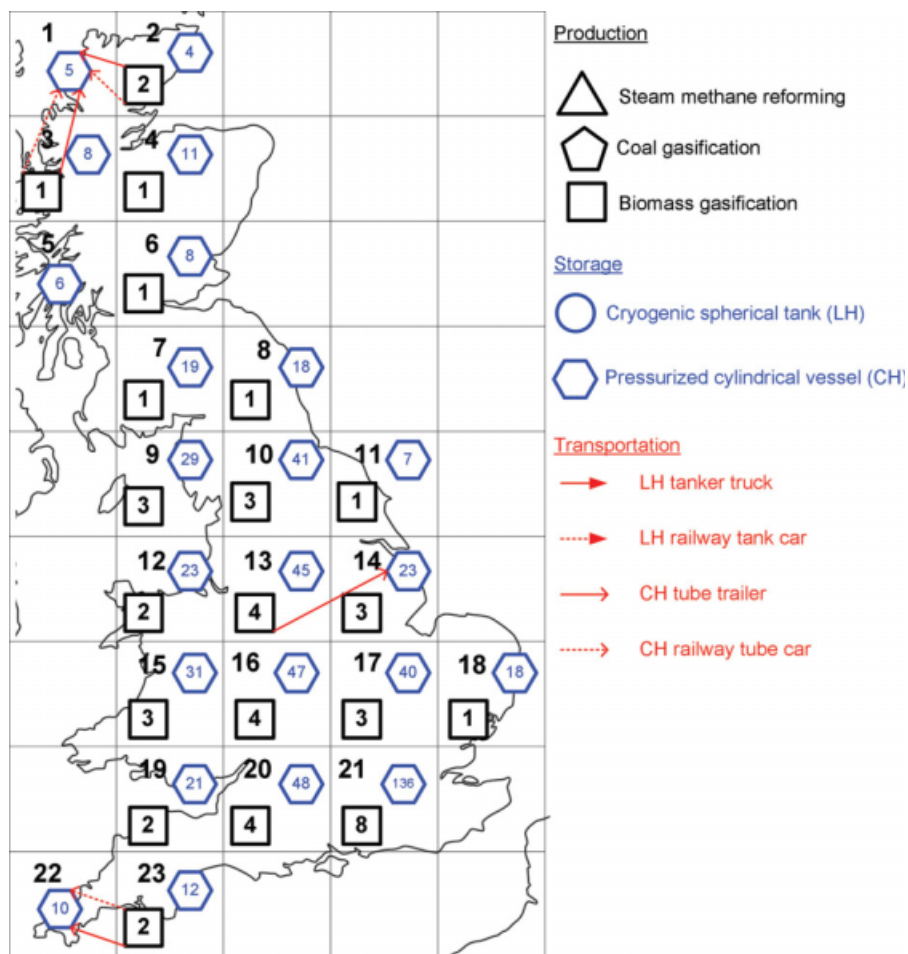
[Color figure can be viewed in the online issue, which is available at [www.interscience.wiley.com](http://www.interscience.wiley.com).]

solution C, compressed hydrogen gas is selected, whereas in option D, part of the hydrogen is transported and stored as a liquid and another part as a gas. In the solution that causes the least environmental impact (E), only compressed hydrogen gas is used. As can be seen, the Pareto curve is rather smooth in the region that goes from A to C, whereas from C to E the slope increases drastically and the shape of the curve becomes sharp.

These results suggest that the most promising alternative to achieve significant environmental savings without compromising too much the total cost of the network is to replace steam reforming by biomass gasification (structural solution B). On the other hand, substituting liquid hydrogen by compressed gas hydrogen does not seem to be a good choice, since this alternative significantly increases the total cost of the hydrogen SC without reducing to a large extent the associated environmental impact. For instance, the environmental impact of solution C is  $6 \times 10^5$  DALYs lower than that of A, whereas its cost doubles approximately that of A. On the other hand, the shift from C to E leads to a reduction of only  $1 \times 10^4$  DALYs in the environmental impact, but increases the cost by a factor of 6, when compared to solution C, and by a factor of 10, when compared to A.

Figures 6 and 7 depict the SC configurations of the extreme solutions (the minimum cost and environmental impact alternatives). The figure also provides the number and type of production plants and storage facilities established in each grid along with the associated transportation links between them. It can be observed that the regions of UK with high population density, mainly Manchester and London (grids 10 and 17, respectively), have higher number of production plants and storage facilities than those with low hydrogen demand. The figures also show that there is at least one storage facility installed in every grid, while the same is not true for the manufacturing plants. Particularly, no manufacturing plant is opened in grids 1 and 22, in which the demand is satisfied by importing hydrogen from other neighboring grids.

It can also be found that the minimum environmental impact solution has more production plants than the minimum cost one (i.e., 50 vs. 36). Furthermore, in the former solution 97.66% of the overall demand is fulfilled by local production, whereas in the latter this percentage drops to 92.20%. These results indicate that the former alternative represents a slightly more decentralized network (i.e., more plants are established). This is because the establishment of more production



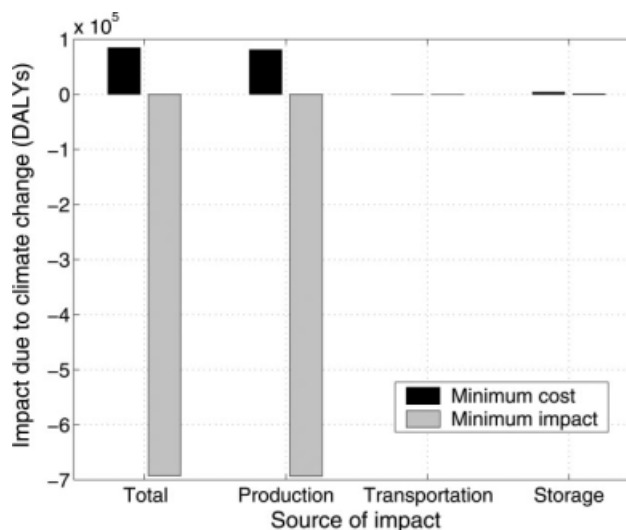
**Figure 7. Minimum environmental impact solution.**

[Color figure can be viewed in the online issue, which is available at [www.interscience.wiley.com](http://www.interscience.wiley.com).]

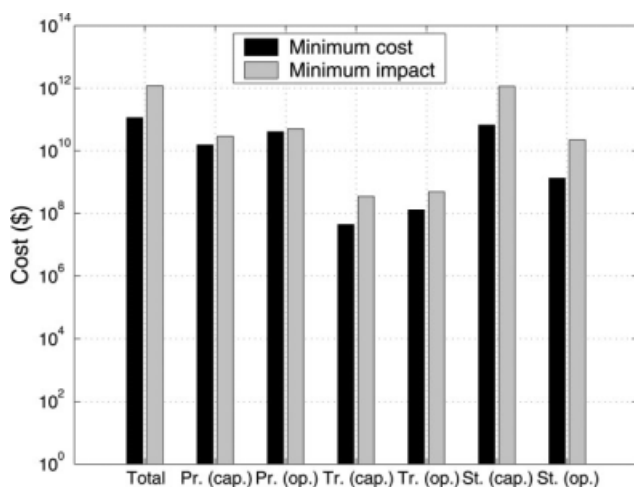
facilities reduces the flow of materials between grids and consequently the emissions associated with the transportation tasks. On the other hand, this policy also increases the capital cost of the SC as it does not fully exploit the concept of economies of scale, and for this reason is not adopted to the same extent in the most profitable solution.

Note also that in the minimum cost solution, hydrogen is stored and transported as a liquid, whereas in the minimum environmental impact alternative, compressed hydrogen is employed. This result may seem surprising, since the capacity of the transport container is about 20 times higher for liquid hydrogen than for compressed gas. This may eventually lead to an increase in the number of trips required between production plants and storage facilities and therefore to higher emissions of greenhouse gases. Note, however, that the energy associated with the liquefaction of hydrogen is much higher than that associated with the generation of compressed hydrogen gas. As commented before, the transportation tasks are minimized in the more sustainable solution by building the plants as close as possible to the markets. Hence, in practice, the latter effect (i.e., energy consumed for compressing hydrogen) compensates the former one (i.e., emissions of the transportation tasks) from the environmental point of view. Unfortunately, from an eco-

nomics perspective, this policy is not appealing at all, since replacing liquid hydrogen by compressed gas hydrogen leads to very large capital costs.



**Figure 8. Main sources of impact.**



**Figure 9. Breakdown of total cost into production (Pr.), transportation (Tr.) and storage (St.) capital (cap.) and operating (op.) costs for the extreme Pareto solutions.**

The extreme solutions also differ in the manufacturing technology employed to produce hydrogen (i.e., steam reforming for the minimum cost alternative and biomass gasification in the minimum impact one). These results can be explained by the low cost of the steam methane reforming and low environmental impact of the gasification of biomass.

Figure 8 shows the contribution of the different sources of impact to the total environmental damage for the extreme Pareto solutions. In the minimum cost solution, the main source of impact is the production of hydrogen. In the minimum environmental impact solution, the main positive contribution to the total impact is the compression of hydrogen. Note that in the latter case the production of hydrogen leads to an impact contribution with a negative sign. This is because, according to the system boundaries settings of our LCA analysis, producing hydrogen from biomass has the environmental advantage of reducing the CO<sub>2</sub> emissions over the entire life cycle of the process.<sup>3,36,37</sup> Particularly, in this solution the carbon sequestration capacity of the biomass feedstock (i.e., wood) compensates the green house gases emissions associated with the SC operation. As can be seen, in both cases the impact due to the transportation and storage tasks is rather small in comparison with that associated with the generation of hydrogen. These results are in consonance with those shown in Figure 5, and explain why substituting the original storage and transportation technologies by others that cause less impact does not reduce significantly the overall environmental damage.

A breakdown of the total cost of each extreme solution is given in Figure 9. As can be observed, in both cases the main contributor to the total cost is the storage capital cost. Furthermore, in the minimum impact solution these costs are approximately one order of magnitude larger than in the minimum cost alternative, and so is the total discounted cost of the network. This is because the unit storage cost for liquid hydrogen is much lower than that associated with a pressure vessel (18 \$ kg<sup>-1</sup> vs. 281 \$ kg<sup>-1</sup>).<sup>35</sup> These data also explain the sharp change that occurs in the shape of the Par-

eto curve when switching from liquid hydrogen to compressed gas hydrogen. On the other hand, the transportation cost represents the smallest contribution to the total cost, mainly because both networks have a high level of decentralization (above 90%). Note that this cost analysis agrees with the economic results obtained by Almansoori and Shah.<sup>19</sup>

## Conclusions

This work has addressed the optimal design and planning of sustainable hydrogen supply chains for vehicle use. The design task was formulated as a bi-criterion MILP problem that seeks to minimize cost and environmental impact. The environmental impact was holistically measured over the entire life cycle of the process by applying the Eco-indicator 99 methodology, which follows the principles of LCA. A decomposition strategy that exploits the mathematical structure of the model was also introduced to expedite its solution.

The capabilities of the proposed modeling framework and solution strategy were shown through a case study based on a real scenario. On the computational side, our solution technique proved to be approximately one order of magnitude faster than the full-space method. Furthermore, the Pareto solutions calculated by our algorithm provided valuable insights into the design problem and suggested process alternatives that may lead to significant environmental improvements. Specifically, from the obtained results it can be concluded that significant reductions in the contribution to global warming can be achieved by replacing steam reforming by biomass gasification. Furthermore, we also observed that decentralized hydrogen networks in which the transportation tasks are minimized lead to lower environmental impacts. These recommendations are intended to guide decision-makers towards the adoption of more sustainable alternatives.

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## Notation

### Indices

- $b$  = environmental burdens
- $i$  = hydrogen form
- $g$  = grid zones
- $l$  = transportation mode
- $p$  = manufacturing technologies
- $s$  = storage technologies
- $t$  = time period

### Sets

- $IL(l)$  = set of hydrogen forms that can be transported via transportation mode  $l$
- $IS(s)$  = set of hydrogen forms that can be stored via technology  $s$
- $IP(p)$  = set of hydrogen forms that can be produced by manufacturing technology  $p$



$PI(i)$  = set of manufacturing technologies that can produce hydrogen form  $i$   
 $LI(i)$  = set of transportation modes that can transport hydrogen form  $i$   
 $SI(i)$  = set of storage technologies that can store hydrogen form  $i$

### Parameters

$av_l$  = availability of transportation mode  $l$   
 $cc_{lt}$  = capital cost of transport mode  $l$  in period  $t$   
 $cud_{lt}$  = maintenance cost of transportation mode  $l$  in period  $t$  per unit of distance traveled  
 $\overline{D}_{gt}$  = total demand of hydrogen in grid  $g$  in period  $t$   
 distance $_{gg'}$  = average distance traveled between grids  $g$  and  $g'$   
 $dsat$  = demand satisfaction level to be fulfilled  
 $fuel_c$  = fuel consumption of transportation mode  $l$   
 $fuelp_{lt}$  = price of the fuel consumed by transportation mode  $l$  in period  $t$   
 $ge_{lt}$  = general expenses of transportation mode  $l$  in period  $t$   
 $ir$  = interest rate  
 $lutime_l$  = loading/unloading time of transportation mode  $l$   
 $\overline{PC}_p^{PL}$  = upper bound on the capacity expansion of manufacturing technology  $p$   
 $\overline{PC}_p^{PL}$  = lower bound on the capacity expansion of manufacturing technology  $p$   
 $\overline{QC}_{gg't}$  = upper bound on the flow of materials between grids  $g$  and  $g'$  via transportation model  $l$   
 $\underline{QC}_{gg't}$  = lower bound on the flow of materials between grids  $g$  and  $g'$  via transportation model  $l$   
 $\overline{SC}_s^{ST}$  = upper bound on the capacity expansion of storage technology  $s$   
 $\underline{SC}_s^{ST}$  = lower bound on the capacity expansion of storage technology  $s$   
 $speed_l$  = average speed of transportation mode  $l$   
 $tcap_l$  = capacity of transport mode  $l$   
 $UB_{gpt}^{PL}$  = upper bound on the number of plants of type  $p$  installed in grid  $g$  in period  $t$   
 $UB_{gst}^{ST}$  = upper bound on the number of storage facilities of type  $s$  installed in grid  $g$  in period  $t$   
 $UB_{lt}^{TR}$  = upper bound on the number of transportation units of type  $l$  purchased in period  $t$  (integer variable)  
 $upc_{igpt}$  = unit production cost of hydrogen form  $i$  produced via technology  $p$  in grid  $g$  in period  $t$   
 $usc_{igst}$  = unit storage cost of hydrogen form  $i$  stored via technology  $s$  in grid  $g$  in period  $t$   
 $wage_{lt}$  = driver wage of transportation mode  $l$  in period  $t$   
 $\alpha_{gpt}^{PL}$  = fixed investment term associated with manufacturing technology  $p$  installed in grid  $g$  in period  $t$   
 $\alpha_{gst}^{ST}$  = fixed investment term associated with storage technology  $s$  installed in grid  $g$  in period  $t$   
 $\beta_{gpt}^{PL}$  = variable investment term associated with manufacturing technology  $p$  installed in grid  $g$  in period  $t$   
 $\beta_{gst}^{ST}$  = variable investment term associated with storage technology  $s$  installed in grid  $g$  in period  $t$   
 $\omega_{bp}^{PR}$  = emissions of chemical  $b$  associated with the production of one unit of hydrogen via technology  $p$   
 $\omega_{bi}^{ST}$  = emissions of chemical  $b$  associated with the compression of one unit of hydrogen into physical form  $i$   
 $\omega_{bl}^{TR}$  = emissions of chemical  $b$  per unit of mass transported one unit of distance with technology  $l$   
 $\theta$  = average storage period  
 $\tau$  = minimum desired percentage of the capacity that must be utilized  
 $v_b$  = damage factor associated with product  $b$

### Variables

$C_{gpt}^{PL}$  = capacity of manufacturing technology  $p$  in grid  $g$  in period  $t$   
 $C_{gst}^{ST}$  = capacity of storage technology  $s$  in grid  $g$  in period  $t$   
 $CE_{gpt}^{PL}$  = capacity expansion of manufacturing technology  $p$  in grid  $g$  in period  $t$   
 $CE_{gst}^{ST}$  = capacity expansion of storage technology  $s$  in grid  $g$  in period  $t$

$D_{igt}$  = amount of hydrogen form  $i$  distributed in grid  $g$  in period  $t$   
 DAM = damage in human health due to climate change  
 $FC_t$  = fuel cost in period  $t$   
 $FCC_t$  = facility capital cost in period  $t$   
 $FOC_t$  = facility operating cost in period  $t$   
 $GC_t$  = general cost in period  $t$   
 $LC_t$  = labor cost in period  $t$   
 $LCI_b$  = life cycle inventory of emissions of chemical  $b$   
 $MC_t$  = maintenance cost in period  $t$   
 $N_{gpt}^{PL}$  = number of plants of type  $p$  installed in grid  $g$  in period  $t$  (integer variable)  
 $N_{gst}^{ST}$  = number of storage facilities of type  $s$  installed in grid  $g$  in period  $t$  (integer variable)  
 $N_{lt}^{TR}$  = number of transportation units of type  $l$  purchased in period  $t$  (integer variable)  
 $PR_{igpt}$  = production of hydrogen mode  $i$  via technology  $p$  in period  $t$  in grid  $g$   
 $Q_{igg't}$  = flow of hydrogen mode  $i$  via transportation mode  $l$  between grids  $g$  and  $g'$  in period  $t$   
 $S_{igst}$  = amount of hydrogen in physical form  $i$  stored via technology  $s$  in grid  $g$  in period  $t$   
 $TC_t$  = total amount of money spent in period  $t$   
 $TCC_t$  = total transportation capital cost in period  $t$   
 $TDC$  = total discounted cost  
 $TMC_{lt}$  = transportation capital cost of mode  $l$  in period  $t$   
 $TOC_t$  = transportation operating cost in period  $t$   
 $X_{gg't}$  = binary variable (1 if a link between grids  $g$  and  $g'$  using transportation technology  $l$  is established, 0 otherwise)

### Literature Cited

- Hugo A, Rutter P, Pistikopoulos E, Amorelli A, Zoia G. Hydrogen infrastructure strategic planning using multi-objective optimization. *Int J Hydrogen Energy*. 2005;30:1523–1534.
- Dunn S. Hydrogen futures: toward a sustainable energy system. *Int J Hydrogen Energy*. 2002;27:235–264.
- Natural Resources Canada, Office of Energy Efficiency. The addition of coal and biomass to hydrogen pathways to GHGenius. Technical Report, 2003, Ottawa, Canada.
- Arnason B, Sigfusson T. Iceland—a future hydrogen economy. *Int J Hydrogen Energy*. 2000;25:389–394.
- Anonymous. Tiny South Pacific Nation leads renewables revolution. *Environ News Service*. 5 October, 2000. Available at: www.hydrogenpacific.com. Last accessed on 13 September 2000.
- Koppel T. Renewable energy in the island state. *Refocus*. 2001; June:1–5.
- Vaitheeswaran V. The slumbering giants awake. A brighter future? A survey of energy. *Economist*. 2001; February: 6–11.
- Myers N, Kent J. *Perverse Subsidies: How Tax Dollars can Undercut the Environment and the Economy*. Washington, DC: Island Press, 2001: 85.
- Ogden J, Williams R, Larson E. A societal lifecycle cost comparison of cars with alternative fuels/engines. *Energy Policy*. 2004;7–27.
- Anonymous. The fuel cell's bumpy ride. *The Economist*. 2001;24 March:39–43.
- Jensen M, Ross M. The ultimate challenge: developing an infrastructure for fuel cell vehicles. *Environment*. 2000;42:10–22.
- Ogden J, Steinbugler M, Kreutz T. A comparison of hydrogen, methanol and gasoline as fuels for fuel cell vehicles: implications for vehicle design and infrastructure development. *J Power Sources*. 1999;9:14–168.
- Ogden J. Prospects for building a hydrogen energy infrastructure. *Annu Rev Energy Environ*. 1999;24:227–279.
- Guy K. The hydrogen economy-developing the infrastructure. In: *Proceedings of the 6th World Congress of Chemical Engineering*, Melbourne, 2001.
- Joffe D, Hart D, Bauen A. Modelling of hydrogen infrastructure for vehicle refuelling in London. *J Power Sources*. 2004;131:13–22.
- Thomas C, Kuhn I, James D, Lomax F, Baum G. Affordable hydrogen supply pathways for fuel cell vehicles. *International J Hydrogen Energy*. 1998;23:507–516.

17. Simbeck D, Chang E. Hydrogen supply: cost estimate for hydrogen pathways—Scoping analysis. Technical Report. Subcontractor report prepared for the National Renewable Energy Laboratory, 2002, Golden, Colorado, USA.
18. van den Heever SA, Grossmann IE. A strategy for the integration of production planning and reactive scheduling in the optimization of a hydrogen supply network. *Comput Chem Eng.* 2003;27:1813–1839.
19. Almansoori A, Shah N. Design and operation of a future hydrogen supply chain. *Chem Eng Res Des.* 2006;84:423–438.
20. Kim J, Lee Y, Moon I. Optimization of a hydrogen supply chain under demand uncertainty. *Int J Hydrogen Energy.* 2008;33:4715–4729.
21. Kim J, Moon I. Strategic design of hydrogen infrastructure considering cost and safety using multi-objective optimization. *Int J Hydrogen Energy.* 2008;33:5887–5896.
22. Li Z, Gao D, Chang L, Liu P, Pistikopoulos E. Hydrogen infrastructure design and optimization: A case study of China. *Int J Hydrogen Energy.* 2008;33:5275–5286.
23. Melo M, Nickel S, da Gama FS. Facility location and supply chain management — A review. *Eur J Oper Res.* 2009;196:401–412.
24. Shapiro JF. *Modeling the Supply Chain.* Pacific Grove, CA: Duxbury Press, 2001.
25. Guillén-Gosálbez G, Caballero J, Jiménez L. Application of life cycle assessment to the structural optimization of process flowsheets. *Ind Eng Chem Res.* 2008;47:777–789.
26. Guillén-Gosálbez G, Grossmann I. Optimal design and planning of sustainable chemical supply chains under uncertainty. *AIChE J.* 2009;55:99–121.
27. Azapagic A, Clift R. The application of life cycle assessment to process optimisation. *Comput Chem Eng.* 1999;10:1509–1526.
28. Hugo A, Pistikopoulos EN. Environmentally conscious long-range planning and design of supply chain networks. *J Cleaner Prod.* 2005;13:1471–1491.
29. Ehrgott M. *Multicriteria Optimization.* Heidelberg, Germany: Springer Berlin, 2005.
30. Dua V, Pistikopoulos E. Parametric optimization in process systems engineering: theory and algorithms. *Proc Indian Nat Sci Acad.* 2003;69:429–444.
31. Iyer RR, Grossmann IE. A bilevel decomposition algorithm for long-range planning of process networks. *Ind and Eng Chem Res.* 1998;37:474–481.
32. Balas E, Jeroslow R. Canonical cuts on the unit hypercube. *SIAM J Appl Math.* 1972;23:61–79.
33. Raman R, Grossmann IE. Relation between MILP modeling and logical Inference for chemical process synthesis. *Comput Chem Eng.* 1993;17:909–915.
34. Amos WA. Costs of storing and transporting hydrogen. Technical Report. National Renewable Energy Laboratory (NREL/TP-570–25106), 1998.
35. Spath PL, Mann MK. Life cycle assessment of hydrogen production via natural gas steam reforming. Technical Report, National Renewable Energy Laboratory (NREL/TP-570–27637), 2001, Golden, Colorado, USA.
36. Koroneos C, Dompros A, Roubas G, Moussiopoulos N. Hydrogen production from Fossil Fuels – A Life Cycle Analysis approach. In: *Proceedings of the International Hydrogen Energy Congress and Exhibition IHEC 2005.* Istanbul, Turkey, 2005: 13.
37. PRé-Consultants. SimaPro 6 LCA software. The Netherlands, 1998. Available at: [www.pre.nl/simapro/default.htm](http://www.pre.nl/simapro/default.htm).
38. PRé-Consultants. The Eco-indicator 99, A damage oriented method for life cycle impact assessment. Methodology Report and Manual for Designers. Technical Report, PRé Consultants, Amersfoort, The Netherlands, 2000.
39. Brooke A, Kendrick D, Meeraus A, Raman R, Rosenthal RE. *GAMS — A User's Guide.* Washington: GAMS Development Corporation, 1998.

## Appendix: Proofs

For convenience in the presentation of the proofs, the objective functions of problems (M) and (UP) are denoted by  $f(\cdot)$  and  $g(\cdot)$ , respectively.

**Proof of Property 1.** Let  $\bar{p}$  be the solution of model (UP) that defines its optimal objective  $g(\bar{p})$ . Assume that there exists a feasible solution  $\bar{q} = (\bar{x}, \bar{X}, \bar{N})$  of (M) such that  $f(\bar{q}) < g(\bar{p})$ . Now, consider the point  $\bar{t} = (\bar{x}, \bar{X}, \bar{RN}, \bar{Z})$ , which has the same vectors of continuous and binary variables  $\bar{x}$  and  $\bar{X}$  as  $\bar{q}$ , and in which the values of  $\bar{RN}$  and  $\bar{Z}$  are defined as follows:

$$\begin{aligned} \overline{RN}_{lt}^{TR} &= \overline{N}_{lt}^{TR} \quad \forall l, t \\ \overline{Z}_{sp}^{PL} &= \begin{cases} 0 & \text{if } \overline{N}_{spt}^{PL} = 0 \\ 1 & \text{otherwise} \end{cases} \quad \forall g, p \\ \overline{Z}_{gs}^{ST} &= \begin{cases} 0 & \text{if } \overline{N}_{gst}^{ST} = 0 \\ 1 & \text{otherwise} \end{cases} \quad \forall g, s \\ \overline{Z}_l^{TR} &= \begin{cases} 0 & \text{if } \overline{N}_{lt}^{TR} = 0 \\ 1 & \text{otherwise} \end{cases} \quad \forall l \end{aligned}$$

Clearly,  $\bar{t}$  is feasible in (UP). Now, from constraints 5 and 9 in (M), we have that:

$$\begin{aligned} \frac{CE_{spt}^{PL}}{PC_p^{PL}} &\leq \overline{N}_{spt}^{PL} \quad \forall g, p, t \\ \frac{CE_{gst}^{ST}}{SC_s^{ST}} &\leq \overline{N}_{gst}^{ST} \quad \forall g, s, t \end{aligned}$$

which implies that the facility capital cost associated with solution  $\bar{t}$  is lower than or equal to that corresponding to  $\bar{q}$ . Since all the remaining terms of  $f(\cdot)$  and  $g(\cdot)$  are the same, we conclude that  $g(\bar{t}) \leq f(\bar{q}) < g(\bar{p})$ . This contradicts that  $\bar{p}$  is the optimal solution of (UP). ■

**Proof of Property 2.** Consider the lower level problems associated with  $W_1^r$  and  $W_1^s$ , which are denoted by  $(LO)^r$  and  $(LO)^s$ , respectively. From the fact that  $W_1^s$  is a subset of  $W_1^r$ , it follows that the right hand side of Eqs. 32–34 in  $(LO)^s$  must be lower or equal than that in  $(LO)^r$ . Since all the remaining equations are the same in both formulations, and Eqs. 32–34 are tighter in  $(LO)^s$ , we conclude that  $(LO)^r$  is a relaxation of  $(LO)^s$ , and therefore yields a valid lower bound on its optimal solution, which implies that  $TDC_{LO}^r \leq TDC_{LO}^s$ . ■

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