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Assessment of mono and multi-objective optimization to design a hydrogen supply chain

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ABSTRACT

This work considers the potential future use of hydrogen in fuel cell electrical vehicles to face problems such as global warming, air pollution, energy security and competitiveness. The lack of current infrastructure has been identified as one of the main barriers to develop the hydrogen economy. This work is focused on the design of a hydrogen supply chain through mixed integer linear programming used to find the best solutions for a multi-objective optimization problem in which three objectives are involved, i.e., cost, global warming potential and safety risk. This problem is solved by implementing an ε-constraint method. The solution consists of a Pareto front, corresponding to different design strategies in the associated variable space. Multiple choice decision making is then recommended to find the best solution through an M-TOPSIS analysis. The model is applied to the Great Britain case study previously treated in the dedicated literature. Mono and multicriteria optimizations exhibit some differences concerning the degree of centralization of the network and the selection of the production technology type.

1. Introduction

Transportation as an economic activity plays a crucial role in the world. Current transport fuels are mainly obtained from oil, considered as a non-renewable fossil fuel, from which gasoline and diesel are produced. The main advantages of producing these fuels are related to existing infrastructure, know-how and experience as well as a huge demand allowing efficiency improvement. Yet, prices in fossil fuel vary in each country and the scarcity of oil reserves constitutes a main concern that may lead to an important increase in the fuel prices. Vehicle industry is trying to improve fuel efficiency and

Abbreviations: CCS, carbon capture and storage; CCF, capital charge factor; FCC, facility capital cost; FCEV, fuel cell electric vehicles; FOC, facility operating cost; GB, Great Britain; GWP, global warming potential; HSC, hydrogen supply chain; ICE, internal combustion engine; LCA, life cycle assessment; LH_2, liquid hydrogen; MCDM, multiple choice decision making; MILP, mixed-integer linear programming; NTU, number of transport units; PCA, principal component analysis; SCM, supply chain management; SMR, steam methane reforming; TCC, transportation capital cost; TDC, total daily cost; TOC, transportation operating cost; TOPSIS, Technique for Order Preference by Similarity to Ideal Situation.

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to decrease pollution since CO_2 tail emissions are responsible for cardiovascular and respiratory diseases as well as for environmental damages such as those impacting construction materials and other surfaces and also those related to affectation in photosynthesis process and smog. To address the threat of climate change, it is necessary to change and to charge a price for carbon emissions. Besides, governments have to do much more, taking actions to support innovation and diffusion of new, low-carbon technologies [1]. In that context, gasoline and diesel production processes have then been reviewed to be less environmental damaging. The transport sector will probably witness a much more diversified portfolio of fuels in the future, with the share of electric mobility in its broadest sense, i.e. electric-drive vehicles powered by a fuel cell, battery, or a hybrid drive train, expected to increase markedly [2]. Future technologies for internal combustion engine (ICE), hybrid electric cars (battery electric cars or plug-in hybrid electric vehicles) and fuel cell electric vehicles (FCEV) are being developed. The use of different fuels constitutes promising alternatives such as biodiesel, methanol, ethanol, methane, liquefied petroleum gas and hydrogen (H_2). Hydrogen which is the most abundant element in the universe and found in compounds of water and hydrocarbons can be extracted to be used as an energy carrier. The projection of hydrogen use in the vehicular system in fuel cells forces to study some elements of the infrastructure that are not yet well developed or established (i.e. storage, transportation and refuelling stations). The study of the so-called hydrogen supply chain (HSC) can help to find different possibilities in the strategic and tactical planning phases for the definition of the H_2 infrastructure. The originality of this study is to take into account sustainable development concepts in early stages of the HSC design. For this purpose, three criteria such as economic, social and environmental impacts are optimized at the same time. The remainder of this paper is organized as follows: the next section presents the advantages and obstacles that may be encountered with the HSC. Then, Section 3 is devoted to a brief review of investigation on HSC. The methodology and objectives of this work are presented in Section 4 where the general elements of the HSC are shown and the mathematical model followed by the definition of a case study in Section 5, results and discussion of mono and multi-objective optimizations are presented in the last section. Finally, conclusions and perspectives are given.

2. General context

Currently, most of the hydrogen is produced in petroleum refineries or in the chemical industry and the most common uses of H_2 are to upgrade fossil fuels and to produce ammonia; it is then usually consumed onsite. Specifically, only about 5% of hydrogen is considered as “marketable” and delivered elsewhere as a liquid or gas by truck or pipeline [3]. Another use of hydrogen is the storage for electricity from intermittent renewable energies, such as wind and photovoltaic energy. When hydrogen is to become a fully-fledged energy carrier, this also implies the use of hydrogen in the residential and commercial sector [4]. Another interesting application of hydrogen and fuel cells is the power supply of portable or remote grid consumers like notebooks or telecommunication devices [5].

Hydrogen offers interesting advantages over competitors; first of all it can be obtained from many energy sources (such as water, biomass, coal, natural gas) and production processes. Fossil fuel sources are the most used nowadays but the implementation of carbon capture and storage (CCS) to steam methane reforming and gasification processes is to be developed. Besides, water electrolysis seems to be the cleaner option when electricity is obtained via renewable energies. In the transport sector well to wheel efficiency of hydrogen as compared to gasoline is higher (about 22–33% vs. 15%) [6]. H_2 has also several potential energy uses (heating homes and offices, to stock renewable electricity, portable applications). Another potential benefit from using hydrogen as transportation fuel can be found in the form of noise reduction[1] in fuel cells.

Reduction in air pollution is also offered by electric cars but several obstacles of use of such vehicles exist such as like the time of the battery recharge, the lack of recharging infrastructure, the high cost associated with the involved lithium battery and perhaps above all a short driving range as compared to ICE or FCEV. Fuel cell technology is well developed and has been rapidly improved in efficiency offering zero emissions at the consumption side. For all these reasons, H_2 seems to be a good candidate as an alternative to the current fossil fuel system because it can help to treat problems like global warming, air pollution, energy security and competitiveness.

However, H_2 faces some obstacles that need to be overcome before being considered as a viable option. The first problem is the lack of infrastructure [8–11], that represents an investment to install a certain capacity large-scale to produce, store and supply hydrogen through a type of technology while at the same time, the lack of demand estimations or projections makes difficult to estimate the required investment. Consequently this interconnected problem blocks the FCEV penetration to the market. The establishment of a new hydrogen infrastructure for fuel cell vehicles is difficult because no smart transition from gasoline or diesel to hydrogen can be expected due to the lack of bivalent operation modes for such vehicles [5]. In this sense, transition would take years. Timing of the investment over the next 10–30 years will also be critical [8]. Most of studies predict an important market penetration of hydrogen in 2050. For Ball and Wietschel [2], hydrogen production and infrastructure costs are not an economic barrier at today’s prices of conventional energy carriers. The critical element is the cost of development of the fuel cell propulsion system, the forecasts being a major source of uncertainty in this case. It is expected that it will take several decades for the build-up of a hydrogen infrastructure and for hydrogen to make a significant contribution to the fuel mix.

Moreover, in some countries, safety norms are focused in the production of H_2 to be used only in chemical processes

[1] This is achieved since the car is powered by an electric motor and thus does not have any of the vibration or exhaust noise created by a typical internal combustion engine vehicle. Some of the effects caused by noise pollution can include hearing loss, cardiovascular problems, and inherent unpleasantness [7].

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with minor transportation and low storage volume. The risk of hydrogen must be considered relative to the common fuels such as gasoline, propane or natural gas; some of H_2 properties make it potentially less hazardous, while other characteristics could theoretically make it more dangerous in given situations [12]. New technologies could be developed or improved to optimize the HSC, then, security norms should be reviewed and implemented in the whole system for using H_2 in vehicles. Comparison between different technology alternatives in the strategic phase is mandatory.

The lack of social or political interest to promote this type of vehicles is another problem; the governments represent an essential part in building the HSC. Environmental regulations and reduction in taxes for the FCEV could help in the introduction phase. Lack of complete scenarios could affect in a bad decision or a disoriented start up in the investment. Without precise assessment, this could represent losses in the total system or at a national project scale.

To study the whole network, tools like supply chain management (SCM) could be applied. Let us recall that supply chain management involves a set of approaches utilized to efficiently integrate suppliers, manufacturers, warehouses, and stores, so that merchandise is produced and distributed at the right quantities, to the right locations, and at the right time, in order to minimize system wide cost while satisfying service level requirements [13]. The focus in SCM can broadly be divided into three main categories, that are design, planning–scheduling and control (real-time management); supply chain models can either be formulated with mathematical programming or with simulation oriented approaches while their application depends on the task in hand. The aim of this paper is to study a general HSC using mathematical programming to design an optimal network so that optimal strategies could be proposed to help decision making.

3. Literature review

The hydrogen supply chain has been studied from different perspectives; first, geographical approaches are devoted to locate the infrastructure elements in a specified area. Second, optimization methodologies are focused on the search for optimal configuration based on a specific objective; third, another approach to design the HSC networks is simulation. A classification of the main studies is presented here to illustrate the current methodologies and case studies:

Some examples of geographical approaches include the study of Ball et al. [14] who developed the MOREHyS (Model for Optimization of Regional Hydrogen Supply) approach of the energy system with the integration of geographical aspects in the analysis by the GIS[2]-based method for Germany.

Johnson et al. [16] used also GIS for modelling regional hydrogen infrastructure deployment using detailed spatial data and applied the methodology to a case study of a potential coal-based hydrogen transportation system in Ohio with CCS. The objective is to optimize hydrogen infrastructure design for the entire state.

Besides, mixed-integer linear programming (MILP) approaches have been widely used for designing the HSC, Almansoori and Shah [17], have clearly introduced a general model that determines the optimal design of a network (production, transportation and storage) for vehicle use where the network is demand-driven. The model was applied to a Great Britain case study. Later, the same authors extended the model in 2009 [18], to consider the availability of energy sources and their logistics, as well as the variation of hydrogen demand over a long-term planning horizon leading to phased infrastructure development as well as the possibility of selecting different scales of production and storage technologies. Other works [19] take into account demand uncertainty arising from long-term variation in hydrogen demand using a scenario-based approach: the model adds another echelon including fuelling stations and local distribution of hydrogen minimizing the total daily cost.

Hugo et al. [8] developed an optimization-based formulation that investigates different hydrogen pathways in Germany. The model identifies the optimal infrastructure in terms of both investment and environmental criteria for many alternatives of H_2 configurations. This model has been extended and considered as a basis for other works such as Li et al. [11] for the case study in China. At the same time in Iran, a model for investigation of optimal hydrogen pathway and evaluation of environmental impacts of hydrogen supply system was examined by Qadrdan et al. [6]. Another study also considered hydrogen from water, using electricity from hydro and geothermal power in Iceland for exportation [20].

Several perspectives of the HSC have been integrated in Kim et al. [10] models as deterministic vs. stochastic approach to consider demand uncertainty in the new model. The model they proposed determines a configuration that is the best for a given set of demand scenarios with known probabilities. The stochastic programming technique used is based on a two-stage stochastic linear programming approach with fixed recourse, also known as scenario analysis. Later, a strategic design of hydrogen infrastructure was developed to consider cost and safety using multi-objective optimization where the relative risk of hydrogen activities is determined by risk ratings calculated based on a risk index method [21].

Guillén Gosálbez et al. [3] proposed a bi-criterion formulation that considers simultaneously the total cost and life cycle impact of the hydrogen infrastructure and to develop an efficient solution method that overcomes the numerical difficulties associated with the resulting large scale MILP. Sabio et al. [22] also developed an approach, which allows controlling the variation of the economic performance of the hydrogen network in the space of uncertain parameters examined the case study of Spain.

More recently, Murthy Konda et al. [9] considered the technological diversity of the H_2 supply pathways together with the spatial–temporal characteristics to optimize a large-scale HSC. They calculate the transportation costs based on Refs. [17] and [18] approaches. The original models are modified (e.g., inclusion of existing plants, capacity expansion and

[2] GIS: Geographical Information System. It is a package that can be usefully integrated with a modelling system for supply chain management. The typical GIS contains an extensive database of geographical census information plus graphical capabilities of displaying maps with overlays pertaining to the company's supply chain activities [15].

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pipeline features) and analysis is extended to incorporate the computation of delivered cost of H_2, well-to-tank emission and energy efficiency analyses. In the work of Haeseldonckx and D'haeseleer [4], the objective is not only to find the optimal set of activated hydrogen production plants but also to implement a hydrogen infrastructure optimization algorithm that has to decide which hydrogen-production plants will be invested in and which plants will not. Finally, Sabio et al. [23] take into account eight environmental indicators in a two-step method based on a combination of MILP multi-objective optimization with a post-optimal analysis by principal component analysis (PCA) to detect and omit redundant environmental indicators.

It can be highlighted that several mono-objective optimization approaches have been developed or extended as in Refs. [6,8,10,14,17–19,24]. In these studies the cost is the objective to be minimized. Multi-objective optimization studies are relatively scarce and criteria to be analyzed are based on economic and environmental performances; some examples are presented in Refs. [3,8,11,23]: minimizing the expected total discounted cost and the associated financial risk [22] and minimizing the total cost of the network and the total relative risk of the network [21].

These works are limited to a bi-criteria assessment, generally based either cost-environment or cost-safety. This is not enough when sustainable development must be taken into account in the strategic stage of any new project, when social, economic and environmental impacts are interconnected: their balance would result in the efficiency of the system. The originality of this study is to consider sustainable development in the HSC design when three criteria such as economic, social and environmental impacts are optimized at the same time.

4. Methodology

In this section, the main principles of the proposed methodology are presented. Firstly, the problem statement, assumptions and objectives are defined with the associated decision variables. The HSC is then presented to establish the general structure of the network. The problem dimension is examined to compare mono and multi-criteria approaches. Finally, the resolution strategy phases are also developed.

4.1. *Problem statement*

As aforementioned, current designs of the HSC reviewed in the dedicated literature are generally based to a multi-objective strategy with two criteria, either cost-environment or cost-safety. A three-criteria optimization model is proposed here considering the interconnection of social, economic and environmental impacts. Their relationship will result in the global balance of the system.

4.1.1. *Objective*

This work will be focused in the design of a three-echelon HSC (production, storage and transportation), considering the minimum cost, the lower environmental impact and the lower safety risk. The model will be tested in a relevant case study (Great Britain) and results for mono-objective optimizations will be compared with the multi-objective solution.

4.1.2. *Given data*

The given data involve hydrogen demand data (each grid has its own deterministic demand), techno-economic, environmental and risk data of the components in the HSC (they are presented in detail in Appendix A, Table A.2).

4.1.3. *Design decisions*

Design decisions are based on the number, type, capacity, and location of production and storage facilities. More precisely, they involve the number and type of transport units required as well as the flow rate of hydrogen between locations. Cities or grids are also considered.

4.1.4. *Operational decisions*

Operational decisions concern the total production rate of hydrogen in each grid, the total average inventory in each grid, the demand covered by imported hydrogen and the H_2 demand covered by local production.

4.1.5. *Assumptions*

- A deterministic demand of hydrogen for the transportation system (particular-light cars and buses) is considered.
- A monoperiod problem is assumed.
- Relative risk of production plant, storage facilities and transportation modes are assumed not to change under the various demand scenarios.
- The model is assumed to be demand driven.

4.2. *Formulation of the HSC*

4.2.1. *General structure of the HSC*

In this formulation, hydrogen can be delivered in specific physical form i, such as liquid or/and gaseous, produced in a plant type with different production technologies p (i.e. steam methane reforming (SMR), biomass or coal gasification); distributed by a specific type of transportation modes l going from the location g to g' referred as grid squares; such that g' is different than g; these grid squares are obtained by dividing the total area of the country or region into n grid squares of equal size, a general HSC is shown in Fig. 1. This supply chain is demand driven and it is a reverse logic network because we assume there are no flows from the market to the facilities or suppliers.

4.2.2. *Supply chain decision database*

Several data are necessary to design the HSC as the base investment and operational costs for a given facility that will be used for extrapolation purpose, the throughput associated with a given technology, the quantities of input and output products associated with unit operations of the transformation types, etc. The whole list is presented in Appendix B.

4.2.3. *Model variables*

The definition of continuous, integer and binary variables is necessary for the mathematical formulation of the HSC

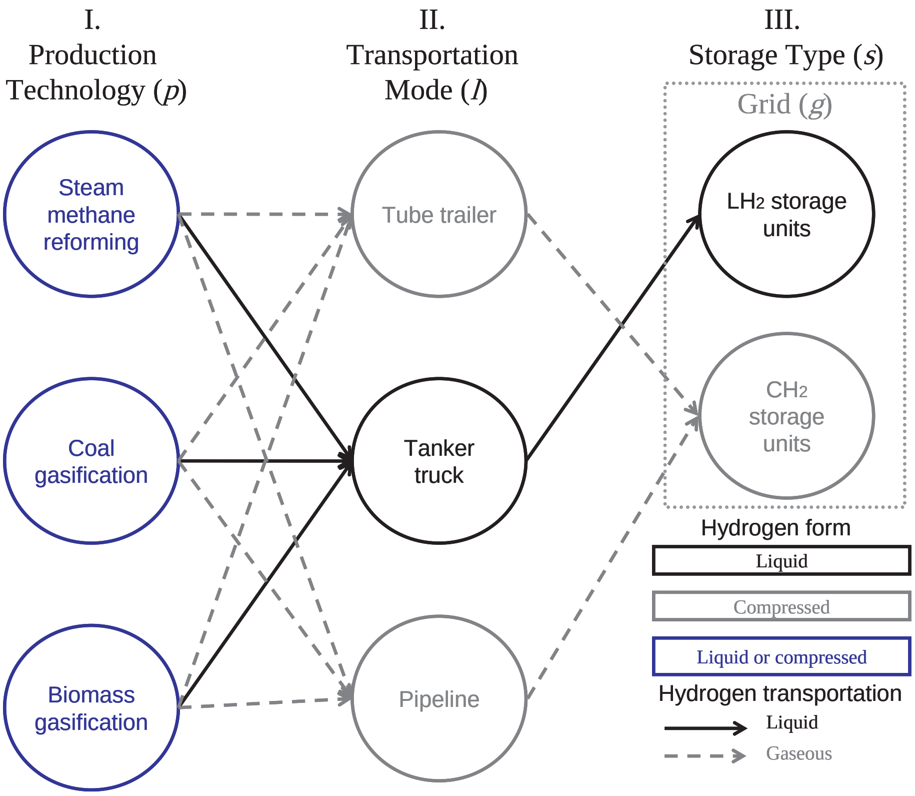

Fig. 1 – A general hydrogen supply chain.

(detailed classification is shown in Appendix A, Table A.3). The problem is then captured in a mixed-integer linear programming (MILP) framework. All continuous and integer variables must be non-negative. Output data will include optimal locations and capacities of new facilities, levels for transformation and process activities at each facility, outbound flows of finished products from production facilities to markets, etc.

4.3. *Mathematical model*

This work is inspired from the previous model of Almansoori and Shah [17]. For reasons of brevity, not all the equations are presented here but mass balance, production, transportation and storage constraints can be found in Appendix A.4 where different constraints features (i.e. equality or inequality, binding and nonbinding) are easily appreciated.

One modification was made to the original model [17]. It consists in the way to calculate the number of transport units (NTU) because it did not take an integer value. Values of transportation capital cost (TCC) and transportation operating cost (TOC) were lower than the real cost considering integer values. Eqs. (1) and (2) were added to the model and Eq. (A.4.16)[3] was modified in Appendix A.4 to allow rounding the NTU value through Eq. (3).

$$V_{ilgg'} \geq 0 \quad \forall i, l, g, g' \tag{1}$$

$$V_{ilgg'} \leq 1 * X_{ilgg'} \quad \forall i, l, g, g' \tag{2}$$

[3] Replaced by Eq. (3) of Section 4.3.

where $V_{ilgg'}$ is a continuous variable with values between 0 and 1 related to the binary value of $X_{ilgg'}$ which takes the value of 1 when the product form i is to be transported from grids g to g'.

Then $NTU_{ilgg'}$ depends significantly on the average distance travelled between different grids ($AD_{gg'}$), the capacity of a transport container ($TCap_{il}$), the flow rate of products between various grids ($Q_{ilgg'}$), the transportation mode availability (TMA_l), the average speed (SP_l), and loading/unloading time (LUT_l). Finally, the $V_{ilgg'}$ is added and an integer value is found.

$$NTU_{ilgg'} = \left(\frac{Q_{ilgg'}}{TMA_l TCap_{il}}\left(\frac{2AD_{gg'}}{SP_l} + LUT_l\right)\right) + V_{ilgg'} \tag{3}$$

4.3.1. *Cost objective*

The total daily cost (TDC) of the network is determined in the same way as in the linear model of Almansoori and Shah [17]. Some comments are given below.

1. Total capital cost – including facilities and transportation modes ($ per day).

   Capital costs for a plant p or a storage facility s are defined as parameters. Then, the costs correspond to the product of the number of new plants and of the number storage units (integer variables) to be installed. Similarly, the transportation capital cost is calculated by multiplying the cost of transport modes by the number of new transport units (integer variable). Both facility and transportation costs are added and divided by the product of the capital change factor (a value of three years is considered as in Ref. [17] and of the network operating period (assumed to be 365 days per year)).

2. Facility operating cost ($ per day).

   This value is constituted by the addition of two terms. The former term corresponds to the product of the unit production cost ($ per kg H_2) and of the average production rate given in kg per day (continuous variable). The latter term is the product of the unit storage cost ($ per kg H_2 per day) and of the average storage rate in kg H_2 (continuous variable).
3. Transportation operating cost ($ per day).

   It is based on the determination of four costs related to transport units:
   - Fuel cost ($ per day) corresponds to the product of fuel price ($ per L) and of the daily fuel usage (L per day); this function takes into account data such as the average distance to be driven, fuel economy, transportation capacity as well as the flow rate of products between various grids (kg per day, as a continuous variable).
   - Labour cost ($ per day) which is obtained by the product of the driver wage ($ per hour) and of the total labour time (hours per day) constituted by the continuous variable of the flow rate of products between various grids (kg per day) and given data such as the transportation capacity (kg per trip), the round trip distance (km), the average speed and the load and unload time of hydrogen (hours).
   - Maintenance cost ($ per day) is defined as the product of maintenance expenses ($ per km) and of the total daily distance driven. It involves the product of the round trip distance (km) and of the continuous variable of the flow rate of products between various grids (kg per day), then divided by the transportation capacity (kg per trip).
   - General cost ($ per day) consists of transportation insurance, license and registration, and outstanding finances. It depends on the integer variable of number of transport units.

   The TDC represents the cost expressed in $ per day of the entire HSC where FCC is the facility capital cost ($), TCC is the transportation capital cost ($), α is the network operating period (days per year) related to the capital charge factor (CCF, in years). Then, the facility operating cost (FOC, $ per day) and the transportation operating cost (TOC, $ per day) are also associated in Eq. (4).

$$\mathrm{TDC} = \left(\frac{\mathrm{FCC} + \mathrm{TCC}}{\alpha \cdot \mathrm{CCF}}\right) + \mathrm{FOC} + \mathrm{TOC} \tag{4}$$

The addition of new constraints to find global warming potential and safety risks values are necessary to implement the proposed multi-objective approach. The definition of the additional objective functions considered is presented below.

4.3.2. *Global warming potential objective*

The global warming potential (GWP) is an indicator of the overall effect of the process related to the heat radiation absorption of the atmosphere due to emissions of greenhouse gases (CO_2-equiv) of the network [25]. The total daily production GWP (PGWP, in g CO_2-equiv per day) is associated with the production rate of product type i produced by each plant of type p in grid g (PR_{pig}, in kg per day) and the total daily GWP in the production facility type p (GW_i^{prod}, in g CO_2-equiv per kg):

$$\mathrm{PGWP} = \sum_{pig} \left(\mathrm{PR}_{pig} \mathrm{GW}_i^{\mathrm{prod}}\right) \tag{5}$$

The total daily storage GWP (SGWP, in g CO_2-equiv per day) is given by Eq. (6) where the PR_{pig} is related to the total daily GWP for the storage technology (GW_i^{stock}, in g CO_2-equiv per kg):

$$\mathrm{SGWP} = \sum_{pig} \left(\mathrm{PR}_{pig} \mathrm{GW}_i^{\mathrm{stock}}\right) \tag{6}$$

The total daily transport GWP (TGWP, in g CO_2-equiv per day) is determined as follows:

$$\mathrm{TGWP} = \sum_{ilgg'} \left(\frac{2\mathrm{AD}_{lgg'} \cdot \mathrm{Q}_{ilgg'}}{\mathrm{TCap}_{il}}\right) \mathrm{GW}_i^{\mathrm{Trans}} \cdot \mathrm{W}_l \tag{7}$$

where the average delivery distance between g and g' by transportation mode l (km trip^{-1}) is multiplied by the flow rate of product form i transported by the mode l between g and g' and divided by the transportation capacity for product form i (kg trip^{-1}). These three terms allow the computation of the number of km per day that must be run to cover the demand taking into account the round trip. Finally those terms are related to the global warming potential (GW_i^{Trans}, in g CO_2-equiv per tonne-km) associated to the transportation mode l and its weight (W_l, in tons).

Eqs. (5)–(7) enable the calculation of the total GWP (GWPTot, in g CO_2-equiv per day) as indicated by:

$$\mathrm{GWPTot} = \mathrm{PGWP} + \mathrm{SGWP} + \mathrm{TGWP} \tag{8}$$

4.3.3. *Safety objective*

Kim and Moon [21,26] developed expressions to evaluate the total risk of production and storage facilities (TPRisk and TSRisk respectively) as well as the total transport risk (TTRisk) where the relative risk of hydrogen activities is determined by risk ratings calculated based on a risk index method. The TPRisk is calculated as follows:

$$\mathrm{TPRisk} = \sum_{pig} \left(\mathrm{NP}_{pig} \cdot \mathrm{RP}_p \cdot \mathrm{WFP}_g\right) \tag{9}$$

where NP_{pig} is the number of plants of type p producing product form i in grid g, RP_p is the risk level of the production facility p and WFP_g is the population weight factor in g in which a production or storage facility is located. The TSRisk is related to the number of storage facilities of type s for products form i in grid g (NS_{sig}), the risk level in storage facility s (RS_s) and the WFP_g as indicated by:

$$\mathrm{TSRisk} = \sum_{sig} \left(\mathrm{NS}_{sig} \cdot \mathrm{RS}_s \cdot \mathrm{WFP}_g\right) \tag{10}$$

The TTRisk is associated with the number of transport units from g to g' ($NTU_{ilgg'}$) in each grid, the safety risk level of transportation mode l (RT_l) and the road risk between grids g and g' ($RR_{gg'}$). The equation adopted in what follows is:

$$\mathrm{TTRisk} = \sum_{ilgg'} \mathrm{NTU}_{ilgg'} \cdot \mathrm{RT}_l \mathrm{RR}_{gg'} \tag{11}$$

By combining Eqs. (9), (10) and (11), the total relative risk (TR) is given by:

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$$TR = TPRisk + TSRisk + TTRisk \tag{12}$$

4.4. Problem dimension

The mono-objective problem dimension treated in Ref. [17] was compared with the multi-objective approach considered in our work to analyze the statistics and main differences (see Table 1). The problem was solved minimizing TDC for both cases but the new constraints presented in Sections 4.3.2 and 4.3.3 were added for the multi-objective case. Then, the number of constraints was doubled and similar results were observed for the number of integer and continuous variables. The computational time increased by a factor of 37% in the multi-objective case. The model dimension involves 12,464 constraints and 6242 variables (among them, 2516 are integer).

4.5. Solution strategy

In a preliminary phase, each mono-criterion problem was optimized separately to analyse how its optimal values are decreased when making a multi-criteria optimization.

4.5.1. *Preliminary phase: mono-objective and lexicographic optimization*

The geographical area (country or region) to be studied is selected and divided in grids or sub-regions. The possible configurations of the HSC to be located in that place are defined (such as product physical form, viable production processes, transportation type, etc....). The mathematical model is then formulated within the GAMS 23.9 [27] environment and solved using CPLEX. Each independent objective function is to be minimized using a lexicographic optimization strategy that produces only efficient solutions when all the objectives are considered.

Mavrotas [28] proposes the use of lexicographic optimization for every objective function in order to construct the payoff table with only efficient solutions. A simple remedy in order to bypass the difficulty of estimating the nadir values of the objective functions is to define reservation values for the objective functions. The reservation value acts like a lower (or upper for minimization objective functions) bound.

Practically, the lexicographic optimization is performed as follows: an objective function (of higher priority) is first optimized, obtaining min TDC = $z1^*$. Then, a second objective function is optimized (total GWP) by adding the constraint TDC = $z1^*$ in order to keep the optimal solution of the first optimization, in order to obtain min GWP = $z2^*$. Subsequently, the third objective function is optimized by adding the constraints TDC = $z1^*$ and GWP = $z2^*$ in order to keep the previous optimal solutions and so on until all the objective functions are treated in a more general case involving more objective functions.

4.5.2. *Solution phase: multi-objective optimization*

The payoff table designed from the application of the lexicographic optimization allows defining the solution. In this approach which tries to minimize all objective functions, the optimal values represent the lower bounds (utopia points) of each objective in the feasible space and the nadir points are relative to values corresponding to the upper bounds on the Pareto surface, and not in any feasible space (values worse than the reservation value are not allowed).

The tri-objective optimization problem is solved by implementing the ε-constraint method. Once the epsilon points (intermediate equidistant grid points) are defined, the objective function TDC has to be minimized. The GWP and TR objective functions are then transformed into inequalities constraints.

The global model can be formulated in a more concise manner as follows:

Minimize {TDC}

$$\begin{array}{l}\text{Subject to :}\\ h(x,y)=0\\ g(x,y)\le 0\\ x\in R^n, y\in Y=\{0,1\}^m, z\in Z^+\\ \text{Risk}=\varepsilon_n(n=0,1,2,\ldots,N)\\ \text{Total GWP}\le\varepsilon_m(m=0,1,2,\ldots,M)\end{array}\quad\left\{\begin{array}{l}\text{Demand satisfaction}\\ \text{Overall mass balance}\\ \text{Capacity limitations}\\ \text{Distribution network design}\\ \text{Site allocation}\\ \text{Cost, environmental and risk correlations}\\ \text{Non-negativity constraints}\end{array}\right\}$$

Table 1 – Statistics for mono and multi-objective approaches.

Type of optimization	Mono-objective	Multi-objective
Number of constraints	6197	12,464
Number of integer variables	1326	2516
Number of continuous variables	1369	3726
CPU time (s)	717	987
Optimal gap (%) 0.01%		

The objective of this formulation is to find values of the operational $x\in R^n$,and strategic $y\in Y = \{0,1\}^m$, $z\in Z^+$ decision variables, subject to the set of equality $h(x,y) = 0$ and inequality constraints $g(x,y) \le 0$. In this model, the continuous operational variables concern decisions dedicated to production, storage and transportation rate, whereas the discrete strategic variables capture the investment decisions such as the selection of activity types and transportation links.

All costs, emissions and risk equations occur as linear functions of the associated decision variables levels. That means the production, storage and transportation costs, GWP

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and safety risk levels are linear values of the associated decision variables. The solution consists of a Pareto front composed of solutions that represent different possibilities of supply chain configurations.

4.5.3. *Multiple choice decision making (MCDM)*

A TOPSIS (*Technique for Order Preference by Similarity to Ideal Situation* [29]) analysis is carried out on the Pareto front with the same weighting factor for the cost, safety and environmental criteria. Then, a modified synthetic evaluation method (M-TOPSIS) [29,30] is also used since it is particularly efficient to avoid rank reversals (unacceptable changes in the ranks of the alternatives [31]) and to solve the problem on evaluation failure that may occur in the original TOPSIS version.

5. Case study

A general HSC is presented in Fig. 1, where the hydrogen form could be liquid or gaseous and some transportation modes and storage facilities are available. A case study of Great Britain (GB) treated by Almansoori and Shah [17] has also been analyzed to illustrate the main capabilities of the new proposed model. GB is divided into 34 grid squares of equal size. Three different production processes are evaluated: SMR, biomass and coal gasification. Hydrogen has to be liquefied before being stored or distributed. Liquid hydrogen (LH_2) is stored in super-insulated spherical tanks then delivered via tanker trucks. Almansoori and Shah [17] estimated the total hydrogen demand in Great Britain as a function of the total number of vehicles, average total distance travelled and vehicle fuel economy (see Appendix B, Table B.1). The estimated demand is assumed to supply private-and-light goods vehicles and buses at 2002 levels. This is based on the assumption that 100% of the abovementioned vehicles would be powered by proton exchange membrane fuel cells (13,392 t per day). Four cases will be analyzed (see Table 2) and compared with those of the *base case* [17]. *Case 1* consists in the minimization of the total daily cost both with a variant approach to compute NTU and a more recent solver version, CPLEX 12 versus CPLEX 9 as the approach used in Ref. [18]. *Case 2* minimizes the total global warming potential (CO_2 emissions) of the network. *Case 3* is devoted to the minimization of safety risk. Finally, Case 4 concerns the simultaneous optimization of the three-abovementioned criteria.

Table 2 – Different case studies and objectives to be analyzed.

Minimization of	Total daily cost	Global warming potential	Total risk
Base case	X		
Case 1	X		
Case 2		X	
Case 3			X
Case 4	X	X	X

5.1. *Techno-economic data*

A large amount of input data is required to solve the problem. All the techno-economic parameters (i.e., minimum and maximum production and storage capacities, average delivery distance between grids and capacity of each transportation mode, etc.) are defined in Appendix B.

5.2. *Environmental data*

As new constraints are integrated to the model, new data were collected to compute the emission of each activity of the supply chain. It must be emphasized that an exhaustive life cycle assessment (LCA studies the impact and effects of a product from the purchase of the raw material until its utilization and elimination. ISO 14040) was not performed. Only CO_2 emissions relative to production, storage and transportation were evaluated. Strømman and Hertwich in Ref. [32] reported that the GWP for the SMR (without CO_2 capture and depository) process was of 10,100 g CO_2-equiv per kg H_2 produced. The same indicator results in 10,540 g CO_2-equiv per kg when hydrogen is produced via coal gasification (underground mined coal) [33]. Biomass gasification leads to 3100 g CO_2-equiv per kg [25]. After liquefaction process, H_2 storage in spherical tanks results in 5251 g CO_2-equiv per kg H_2 according to the Detailed California Modified GREET pathway in 2009 [34] including manufacture, construction facilities, fuel consumption, flare combustion and methane venting. Moreover, an amount of 62 g CO_2-equiv per tonne-km is emitted by tanker truck transportation [35] and the weight of the transportation taken into account is 40 t [36].

5.3. *Safety data*

The evaluation of the safety risk takes as parameters three indicators, i.e., the risk level of each activity, the population weight factor and the adjacency level in transportation links. For the risk level of each activity (H_2 production-storage facilities and transportation units), Kim et al. [21] [26] have developed a risk assessment methodology through the hazard identification using the failure modes and effects analysis (FMEA) and the consequence-likelihood analysis to complete the risk evaluation (each hazard is plotted on a frequency vs. consequence matrix (risk binning matrix), that indicates its level of risk as high, moderate, low, or negligible). The risk-binning matrix in Ref. [21] summarizes the individual risk and relative risk level according to its remark raking and is taking into account for our database. All hydrogen activities considered are marked as Levels II–IV according to harmfulness for people, the environment and facilities. The acceptance criterion of these levels is described in Appendix B, Table B.5. A risk level III corresponds to SMR, tanker truck and liquid storage. Values for biomass and coal gasification were not found, then, they were assumed to have the same risk level as SMR.

The population risk weight factors for each grid are classified in Table 3, i.e., when the population of a particular grid is over 2 millions, we assume that this region has a score of 5, from 1 to 2 millions the score is 4 and so on. According to this

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Table 3 – Relative impact level of grids based on the population density.

Population level (persons per grid)	Grids
Level 1 (under 2.5^{E+05})	2,5,8,9,12,16,20,21,26,34
Level 2 (2.5^{E+05}–5^{E+05})	1,3,4,6,7,15,30,31,32,33
Level 3 (5^{E+05}–1^{E+06})	10,11,17,19,25,27
Level 4 (1^{E+06}–2^{E+06})	13,22
Level 5 (over 2^{E+06})	14,18,23,24,28,29

classification, a higher weighting rate for grids corresponds to a higher population density.

The adjacency level in transportation links was calculated as a function of the crossed grids or those close to the road. If hydrogen is transported through some intermediate grids, the impacts on these regions must be taken into account as indicated in the following equation:

$$RR_{gg'} = \sum_{g} \left(RL_g + \beta_{g2} RL_{g2} + \beta_{g3} RL_{g3} + \ldots + RL_{g'} \right) \quad (13)$$

where subscripts g and g' represent the first and last regions and $g_1, g_2, \ldots, g_n$ represent the intermediate regions through which hydrogen is transported; β_g is the weight factor that indicates the adjacency level of a region in which the route is located. It takes a rating value between 0.1 and 1.0 according to the adjacency level. For a transiting grid, the value is 1, for a close region, the value is 0.5, this value is multiplied by the risk level of the grid (RL_g, see Table B.6) classified according to the grid size – by population density (i.e., small = 1, medium = 2 or large = 3). This calculation is detailed in the method proposed by Kim and Moon [26]. Due to the geographical division of the original case study [17], some difficulties were encountered to precisely locate the roads. The following method was then adopted: if hydrogen produced in region 1 is transported to region 33, this transportation arc has to penetrate nine grids ($g1$, $g4$, $g7$, $g10$, $g13$, $g17$, $g23$, $g28$ and $g33$) and is close to four grids ($g2$, $g3$, $g18$ and $g22$); applying Eq. (13), the external effect factor of the transportation arc from region 1 to 33 is 25.5 (see Table B.6). Appendix B, Table B.4 shows the total relative risk matrix for impact on city transportation between grids. The highest risk line is the hydrogen transportation from grid 31 (565) and the lowest risk line concerns hydrogen transportation from grid 17 (335). If decision-makers design the hydrogen supply chain by considering only transportation safety, it is safer to completely avoid transportation from grid 31.

6. Results and discussion

The different stages of the proposed methodology were developed and applied in the abovementioned case study. In this section, the results and corresponding configurations are analysed and discussed in detail. In a preliminary phase, the three criteria were optimized separately to analyse how their optimal values decrease when making a multicriteria optimization. The ε-constraint method is applied and the best compromise solution is then chosen from the Pareto front via M-TOPSIS.

6.1. *Preliminary phase*

The preliminary phase allowed finding the payoff table through lexicographic optimization (see Section 4.5). Thus, it is possible to obtain as the solution that minimizes TDC as the one that corresponds to point that is a non-dominated solution also for total GWP and total risk. The optimization runs were performed for *cases* 1, 2 and 3 where cost, CO_2 emissions and safety risk are to be minimized. The results of each independent optimization can be seen in Table 4. The optimization runs were implemented with a Pentium (R) Dual-core CPU E6600@3.06 GHz processor machine.

Following the conventional optimization we first calculate the payoff table by simply calculating the individual optima of the objective functions. The conventional MILP optimizer will produce the payoff table shown in Table 4(a). However, it is almost sure that a conventional MILP optimizer will calculate the solution of the first point and will stop the searching giving this solution as output. In order to avoid this situation, the

Table 4 – Comparison between conventional (mono-objective) and lexicographic optimization results.

	(a) Payoff table obtained by a **conventional** MILP optimizer			(b) Payoff table obtained by the **lexicographic** optimization		
Case	1	2	3	1	2	3
Minimize	TDC	GWP	TR	TDC	GWP	TR
Total network cost M($ per day)	**64.57**	135.92	77.57	**64.57**	132.05	73.65
Total GWP (10^3 t CO_2-equiv per day)	205.86	**111.85**	203.35	205.86	**111.85**	205.6
Total risk (units)	10,363	6005	**5970**	10,292	5970	**5970**

TDC: total daily cost.
GWP: global warming potential.
TR: total risk.

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lexicographic optimization of the objective functions is performed and the results are shown in Table 4(b). It can be highlighted that the optimal solution obtained through conventional optimization of TDC (TDC = 64.57 M$ per day, total GWP = 205.86 × 10^3 t CO_2-equiv per day and total risk = 10,363 units) is a dominated solution in the problem due to alternative optima resulted through the lexicographic optimization (TDC = 64.57 M$ per day, total GWP = 205.86 × 10^3 t CO_2-equiv per day and total risk = 10,292 units); the total risk is decreased by 71 units. The same analysis can be made for the two other objective functions. The bold characters in Table 4 (it will be also the case in Tables 5 and 6) are relative to the value of the optimized criterion for the mono-objective optimization and in the case of the lexicographic optimization is related to the first optimized objective (higher priority).

Information concerning the decision variables is presented in Table 5. The values of flow rates between grids, total production and storage per day in each location can be found in Appendix C. All the mono-objective cases are analysed in the next section.

6.1.1. *Base case and case 1 (minimal TDC)*

The results obtained in *case 1* are in agreement with the *base case* [17]. The minimal number of 28 production plants is obtained with steam methane reforming (SMR) technology dispersed throughout GB territory. Production of LH_2 via SMR has also been found in previous works [23,24], with cost as an objective function. The number of storage units is 265 when adopting the same value for demand and with a storage period of 10 days. *Case 1* involves 171 tanker trucks to cover the demand between grids which represents a transportation capital cost of 85.5 M$ as compared with 80.2 M$ in Ref. [17] where the number of transport units is not reported. Transportation costs (i.e., fuel, labour, maintenance and general costs) are directly influenced by the number of trips, trip distances and number of transport units for each case. Among all the case studies, the higher transportation cost is observed for *case 1* when minimizing TDC: less plants are installed but more transport units are required to cover all the national demand, consequently, the transportation operating cost is also higher and the network results in a centralized HSC with the minimal total daily cost for the network of 64.57 M$.

The configurations that can be obtained are presented in Figs. 2 and 3 and exhibit low differences in the distribution links and liquid hydrogen amounts to be transported between *base case* and *case* 1. The minor variations that can be observed could be attributed to the solver version. In *case* 1, less distribution links are found but the amount of LH_2 transported keeps the same value. The imported part of demand of LH_2 between grids and the flow rates is listed in Appendix C, Table C.2.

Table 5 – Mono-objective and lexicographic optimization results of the hydrogen supply chain.

Case		Base case [17]	1	2	3
Minimization of		Cost	Cost	GWP	Risk
Decisions	Number of production facilities	28	28	47	47
	Number of storage facilities	265	265	265	265
	Number of transport units	–	171	3	3
Criterion 1 "Cost"	*Capital cost*				
	Plants and storage facilities (M$)	47,310	47,310	98,694	57,475
	Transportation modes (M$)	80.22	85.50	1.50	1.50
	Total daily capital cost (M$ per day)[a]	43.28	43.28	90.13	52.49
	Operating cost				
	Plants and storage facilities (M$ per day)	21.16	21.16	41.92	21.16
	Transportation modes (M$ per day)	0.126	0.126	0.001	0.001
	Total operating cost (M$ per day)	21.29	21.29	41.92	21.16
	Total cost				
	Total network cost (M$ per day)	64.57	**64.57**	132.05	73.65
Criterion 2 "Global warming potential (GWP)"	Production facilities (10^3 t CO_2-equiv per day)	–	135.27	41.52	135.27
	Storage facilities (10^3 t CO_2-equiv per day)	–	70.33	70.33	70.33
	Transportation modes (10^3 t CO_2-equiv per day)	–	0.261	0.002	0.002
	Total GWP (10^3 t CO_2-equiv per day)	–	205.86	**111.85**	205.60
Criterion 3 "Total relative risk"	Transportation modes	–	4557	40	40
	Production facilities	–	580	775	775
	Storage facilities	–	5155	5155	5155
	Total risk (units)	–	10,292	5970	**5970**

a Assuming a capital charge factor—payback period of capital investment of 3 years and the network operating value in 365 days per day. Demand 13 392 360 kg per day.

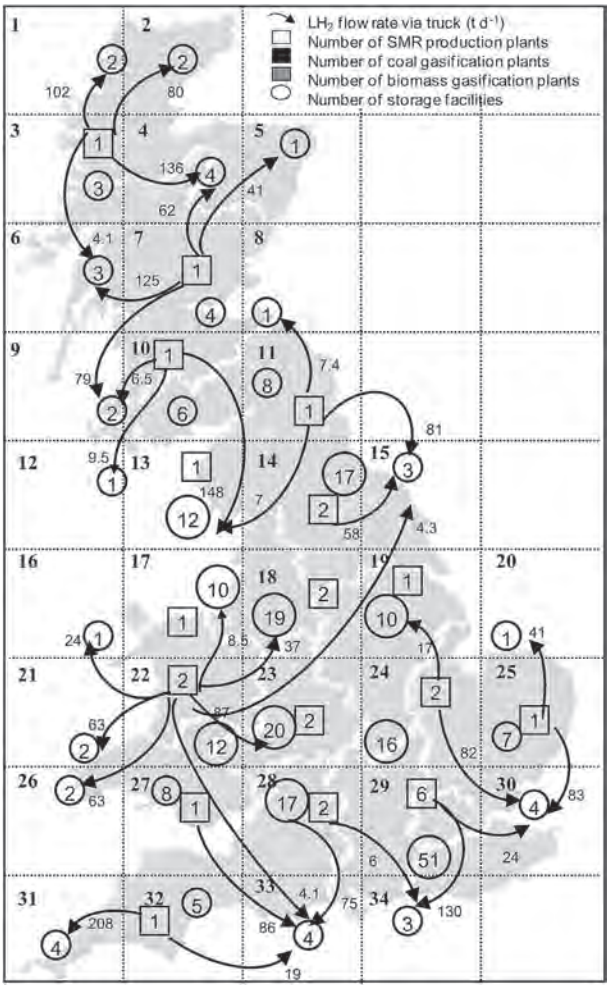

Fig. 2 — Network structure of liquid hydrogen produced via medium-to-large SMR plants, stored in medium-to-large storage facilities, and distributed via tanker trucks. Cost minimization (Almansoori and Shah, 2006).

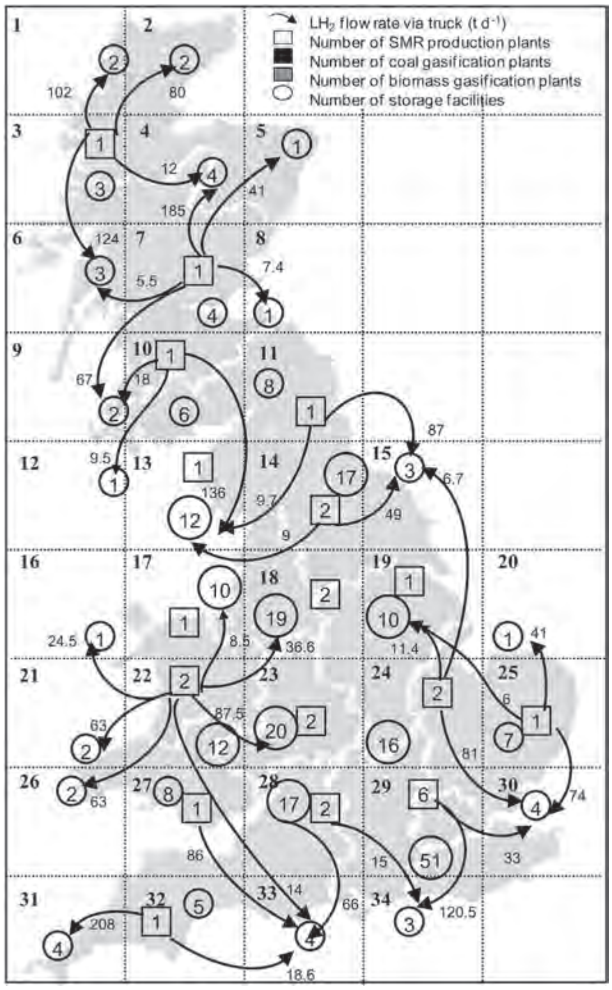

Fig. 3 — Network structure of liquid hydrogen produced via medium-to-large SMR plants, stored in medium-to-large storage facilities, and distributed via tanker trucks for the case 1 (cost minimization).

6.1.2. Case 2 (minimal GWP)

Case 2 is relative to the minimization of the global warming potential. Minimal total GWP resulted in 111.85×10^3 t CO_2-equiv per day in which the main contribution is given by the liquid storage process (62%), followed by the amount emitted by the production facilities (37%) and a minimal impact of transportation (only three tanker trucks are considered in this network). In the case of storage facilities, the solver does not change the amount of facilities installed since there is only one size of storage tank, so that the optimization is only performed with the number of production facilities and transportation units as significant decision variables. The number of production plants increase considerably (from 28 plants in *case 1* to 47 in this case) and all of them are biomass gasification facilities. The kind of technology plays a key role in the CO_2 emissions: biomass gasification technology decreases GWP but represents also a higher investment affecting the total daily cost of the HSC which is more than two times higher compared to the *case 1*. Guillén et al. [3] also found that the most promising alternative to achieve significant environmental savings consisted in replacing SMR by biomass gasification. In Fig. 4, it can be highlighted that only three transportation links are established (from grids 9 to 10, 11 to 8 and from 16 to 17). As mentioned in Guillén et al. [3], *case 2* HSC design results in a decentralized network where almost all the grids are autonomous in LH_2 production.

6.1.3. Case 3 (minimal relative risk)

Case 3 minimizes the total relative risk. The optimal configuration is shown in Fig. 5. Figs. 4 and 5 show similarity in the degree of decentralization with only three distribution links and three tanker trucks assigned for the whole supply chain. Less links and transport units are assigned and are related to a higher number of installed production facilities, which is consistent with the results of *cases 1* and 2. Specific features for *case 3* can be highlighted for production units with a total of 47 facilities located in

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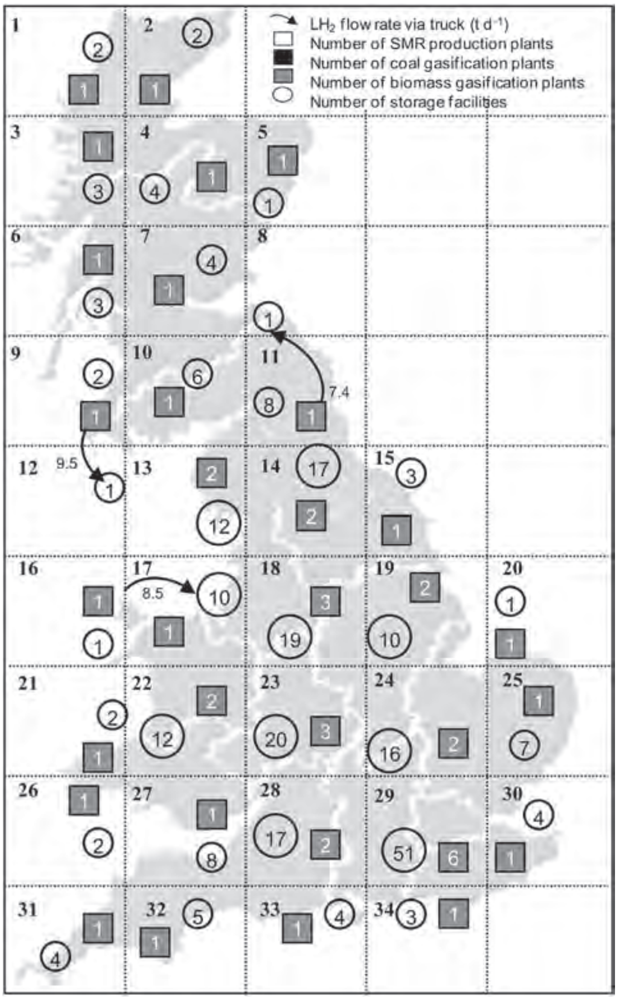

Fig. 4 – Network structure of liquid hydrogen produced via medium-to-large biomass gasification plants, stored in medium-to-large storage facilities, and distributed via tanker trucks for the case 2 (CO_2 minimization).

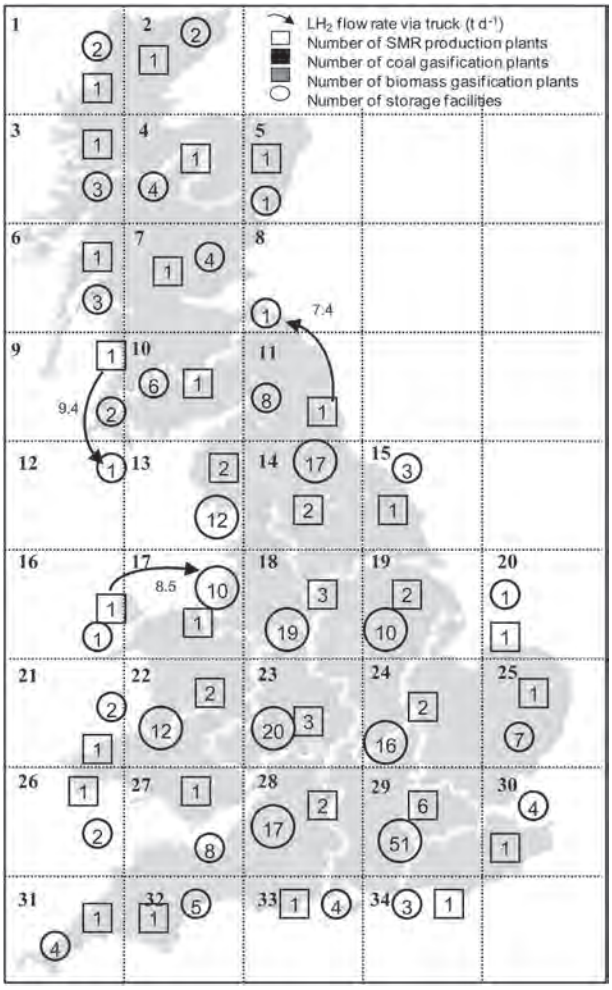

Fig. 5 – Network structure of liquid hydrogen produced via medium-to-large SMR plants, stored in medium-to-large storage facilities, and distributed via tanker trucks for the case 3 (risk optimization).

all the grids except in grid 8 and 12; even though Kim and Moon [26] found that the installation of plants changed in those grids with less population density, this was not found here (i.e. grid 29 involves a total of 6 production units). The main difference between *case 2* and 3 is the production technology which results in 100% of installed SMR plants when risk is minimized.

The total relative risk for this case is of 5970 units and is basically influenced by the storage risk (86%) since storage is scattered in each grid to cover a volume equivalent to 10 days of demand of LH_2 per grid. Yet, from the results of this case study, it cannot be deduced that safety risk will be lower if more small storage units are installed since the different storage sizes were not considered. A variation in the number of storage units was not found. The production risk is the second major risk (13%). The transportation relative risk was reduced to find a more safety configuration considering at the same time the links and distance to be run. It must be pointed out that the number of tanker trucks was dramatically reduced from *case 1* to *cases* 2 and 3 (from 171 to 3 units); in the second case this was made to decrease GWP but in this case the transportation risk represented 44% in *case 1* and represents less than 1% for *case 3*. Through analysis of production plants and the transportation modes, Kim and Moon [21] determined that changing the type of plant or mode does not offer additional financial benefits or safety guarantees. Yet, in our case, we found that the production technology mix of *case 3* represents a financial benefit of 44% as compared to the *second case* where 100% of biomass gasification plants were installed.

6.2. *Multi-objective optimization*

From the three independent mono-objective cases, each objective function range can be obtained so that, the ε-constraint method can be applied. From the lexicographic optimization results of Table 4(b), the utopia and nadir points of each criterion can be found. The total risk can be divided

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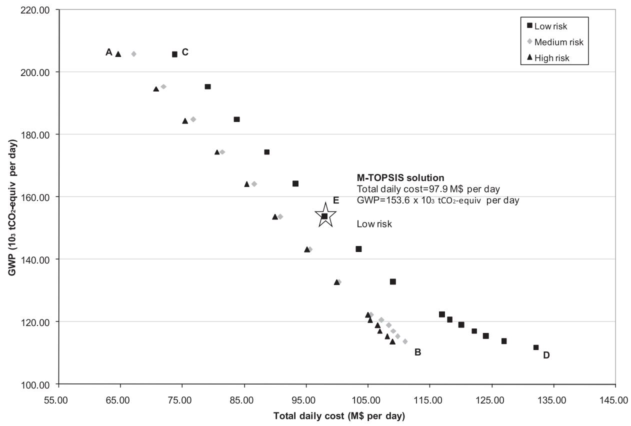

Fig. 6 – Pareto solutions for the multi-objective model.

into three intervals to make the interpretation easier: *low risk* = 5970 corresponding to the best possible obtained, *medium risk* = 8132 (the intermediate value defined by the epsilons ε_n) and *high risk* = 10,292 units corresponding to the nadir point according the payoff table. Similarly, 15 epsilon points were defined for GWP. Then, the objective function TDC has to be minimized while total GWP and total risk are considered as inequality constraints. The solution consists of a Pareto front composed of solutions for supply chain configurations (see Fig. 6). The cost of both *high* and *medium* risks is similar since these two levels of risks have close impacts of CO_2 emissions, that is because of the degree of centralization higher in the *high risk* network and also with longer route links and with more trips per day. This represents a benefice in TDC compared with the *low risk*. In Fig. 6 lines of *medium* and *high* risks options are very close, according to this result if the decision maker prefers to decrease the safety risk from high to medium, this decision will not represent a high cost affectation compared to the investment cost that would be necessary to change from *high* to *low* risk. The degree of decentralization in the *low risk* is the main difference and at the same time the impact of the technology type that impacts directly the cost and the GWP (i.e. the capital cost of establishing biomass gasification plant is of M$ 1412 vs. M$ 535 for the SMR technology [17]). Then if the risk level is to be low and to assure to emit less CO_2 a higher investment is necessary.

Five points are plotted (*A*–*E*) in the Pareto front (see Fig. 6) to give an example of the difference in the degree of decentralization. The point *A* is the most centralized configuration with 36 distribution links and 171 tanker trucks assigned for the whole supply chain. The flow rate for this configuration can be seen in Table C.1. This solution corresponds to a *high risk* with low cost with a maximum of CO_2 emissions. At the same time, the point *B* is connected by 26 links and 115 tanker trucks, similar results are found for the other solutions of *medium risk*. Finally, a low degree of centralization is found for solutions with *low risk*, points *C*–*E* require only 3 transport units to distribute less then 1% of the total daily demand of hydrogen, the remaining part is produced on-site.

The 43 possible set solutions in the Pareto front were evaluated via TOPSIS and M-TOPSIS analysis [29,30] carried out with the same weighting factor for the cost, safety and environmental factors (see Appendix C, Table C.3).

6.2.1. *Case 4 (multi-objective optimization)*

Based on the data and assumptions, the optimal configuration of the future HSC involves 47 production plants as a mix of production technologies (i.e. 66% for SMR and 34% for biomass gasification) located in a decentralized configuration. This network uses tanker trucks to deliver liquid LH_2 to storage facilities. This option involves a TDC of 97.97 M$ per day, a GWPTot of 153.63×10^3 t CO_2-equiv per day and a low safety risk.

Table 6 – Multi-objective optimization results of the hydrogen supply chain.

Case		4
Minimize		Cost, GWP and risk
Decisions	Number of production facilities	47
	Number of storage facilities	265
	Number of transport units	3
Criterion 1 “Cost”	*Capital cost*	
	Plants and storage facilities (M$)	71,507
	Transportation modes (M$)	1.50
	Total daily capital cost (M$ per day)[a]	65.30
	Operating cost	
	Plants and storage facilities (M$ per day)	32.67
	Transportation modes (M$ per day)	0.001
	Total operating cost (M$ per day)	32.67
	Total cost	
	Total network cost (M$ per day)	***97.97***
Criterion 2 “Global warming potential”	Production facilities (10^3 t CO_2-equiv per day)	83.30
	Storage facilities (10^3 t CO_2-equiv per day)	70.33
	Transportation modes (10^3 t CO_2-equiv per day)	0.002
	Total GWP (10^3 t CO_2-equiv per day)	**153.63**
Criterion 3 “Risk”	Transportation modes	40
	Production facilities	775
	Storage facilities	5155
	Total risk (units-level)	**5970**

a Assuming a capital charge factor—payback period of capital investment of 3 years and the network operating value in 365 days per day. Demand 13,392,360 kilos per day.

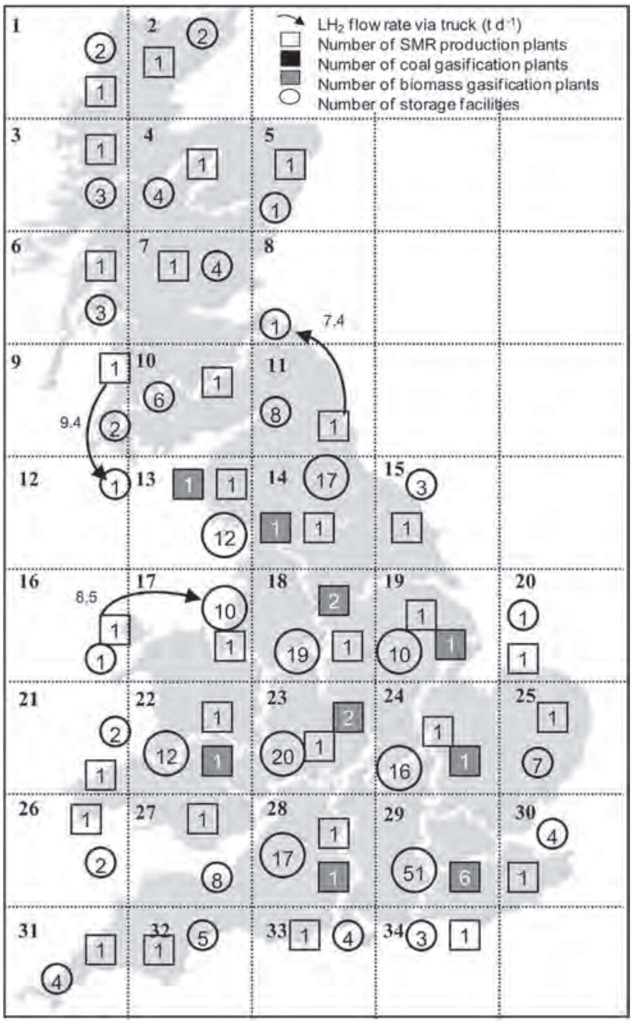

Fig. 7 – Network structure of liquid hydrogen produced via medium-to-large SMR and biomass gasification plants, stored in medium-to-large storage facilities, and distributed via tanker trucks for the case 4 (multi-objective optimization).

The results concerning the decision variables for the multi-objective optimization problems are displayed in Table 6 and Fig. 7 shows the corresponding configuration. The analysis of the network is quite different from the mono-objective configuration of Fig. 3. In the *base case*, it can be observed that long transportation links are installed between grids because such an option is cheaper than building a new production facility. It must be emphasized that the degree of decentralization increases in the multicriteria solution and is similar in cases *2 and 3*.

The change from a centralized to a decentralized supply chain is the main difference observed when the safety risk and the CO_2 emissions are taken into account in the optimization phase. The production plants work with less efficiency because they have a maximum capacity of 480 t per day and in some cases they are producing only 10 t per day. Different plant sizes could be studied in a future approach.

Table 7 shows that the best value obtained for TDC in the multi-objective approach (*case* 4) is higher (an increase by 34% is observed) than for mono-objective case (*case* 1). Moreover, the CO_2 emissions and the risk are improved in *case* 4 reducing GWP by 34% and the total risk by 72%. The total GWP decreases by 27% in *case 2* as compared with *case* 4 while the reduction in CO_2 emissions implies a higher cost (35%) while not affecting the risk. Finally, the minimal risk was found in cases 3 and 4 (best results are shown in Table 4 for the lexicographic optimization) but the other two criteria are different. The TDC increases by 25% in *case* 4 but the CO_2 emissions are decreased by 34% as compared with *case 3*.

Finally, the unitary cost of hydrogen per case is presented in Fig. 8. It must be highlighted that no refuelling station is included in this optimization of the HSC, even though these results could give us an idea about the competitiveness of H_2 with fossil fuels. One kilogram of hydrogen is approximately equivalent to one gallon of gasoline based on its lower heating value energy content [37]. Any hydrogen source that has a hydrogen cost below the current cost of gasoline has an economic advantage over gasoline. Gasoline prices in 2012 are 3.5–4.0 $/gallon (retail price range [38]). According to Ball and Wietschel [2], the specific hydrogen supply costs are estimated at around 4–4.6 $/kg for being representative for both the European Union and North America in the early phase. They are mainly due to the required overcapacity of the supply and refuelling infrastructure as well as to the higher initial costs for new technologies because of the early phase of technology learning. Around 2030, hydrogen costs range from 3.6 to 5.3 $/kg in the abovementioned regions, mainly depending on the feedstock. In the long term until

Table 7 – Results comparison among the treated cases.

	Total daily cost (M$ d^{-1})	Total GWP (10^3 t CO_2-equiv per day)	Total risk (units)
Multi-objective optimization (Case 4)	97.97	153.6	5970
Minimal TDC (Case 1)	64.57	205.86	10,292
Difference between Case 4 vs Case 1	34%	−34%	−72%
Minimal GWP (Case 2)	132.05	111.85	5970
Difference between Case 4 vs Case 2	−35%	27%	0%
Minimal risk (Case 3)	73.65	205,6	5970
Difference between Case 4 vs Case 3	25%	−34%	0%

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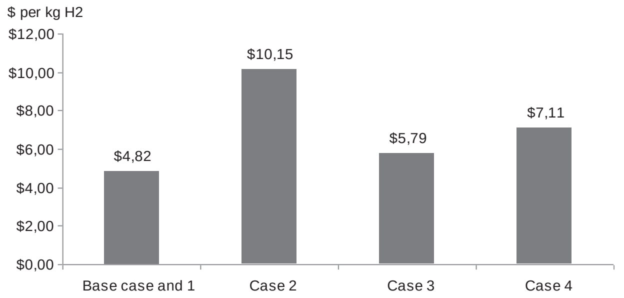

Fig. 8 – Hydrogen cost ($ per kg).

2050, hydrogen supply costs will stabilize around this level, but with an upward trend due to the assumed increase in energy prices and CO_2 certificate prices. The average H_2 delivered cost found in Ref. [8] varies from 4.5 to 6.8 $/kg (prices in 2008). According to these references, it can be concluded that the cost of the HSC defined in this problem is still high for the problem that was considered and it will not be competitive to the current fossil fuel system unless some parameters (e.g. the capital change factor-payback period) are modified.

7. Conclusions and remarks

This paper has presented a general methodology for the design of an HSC using multi-objective optimization. The model developed is an extension of the approach developed in Ref. [17]. In this work, while TDC is minimized, investment strategies have been found for designing a sustainable hydrogen economy based on careful analysis that takes into account other critical issues such as safety and environmental impact. The solution strategy is based on the ε-constraint method as a multi-objective optimization technique for considering three objectives to be minimized simultaneously, involving economic, environmental and safety indicators. From the case study analysis, it must be highlighted that the model can identify the optimal HSC including the number, location, capacity, and type of production, transport and storage facilities, production rate of plants and average inventory in storage facilities, hydrogen flow rate and type of transportation links to be established. The main differences found between the two approaches are related to the degree of the production decentralization that starts to increase as the risk and CO_2 emissions are taken into account. This means that the demand of hydrogen will be supplied by a number of production facilities scattered throughout GB and the number of transport units will decrease under the assumptions made considering no intra grid transport. Production plants resulted only in SMR type for the base case but when multiobjective optimization is performed, a mix of technologies is involved, i.e. SMR and biomass gasification. Some further works are now under investigation in order to improve the model within this scope: demand variation needs to be considered since H_2 is not only required for vehicle use; the energy sources and the fuelling stations nodes to the hydrogen supply chain must be included in the model; a geographical division based on states or regions instead of grid squares would be more realistic to facilitate data collection; the model must be extended to treat a panel of renewable energy sources.

Appendix A. Mathematical model

Table A.1 – Indices.

g: grid squares and g': grid squares such that $g' \neq g$
i: product physical form
l: type of transportation modes
p: plant type with different production technologies
s: storage facility type with different storage technologies

Table A.2 – Parameters.

General data		
DT_{ig}	Total demand for product form i in grid g	kg per day
α	Network operating period	days per year
CCF	Capital change factor – payback period of capital investment	years
WFP_g	Weight factor risk population in each grid	units
Production data		
$PCap_{pi}^{min}$	Minimum production capacity of plant type p for product form i	kg per day
$PCap_{pi}^{max}$	Maximum production capacity of plant type p for product form i	kg per day
PCC_{pi}	Capital cost of establishing plant type p producing product form i	$
UPC^{pi}	Unit production cost for product form i produced by plant type p	$ per kg
GW_p^{Prod}	Production global warming potential by plant type p	g CO_2-equiv per kg of H_2
RP_p	Risk level of the production facility p	units
Storage data		
$SCap_{si}^{min}$	Minimum storage capacity of storage type s for product form i	kg
$SCap_{si}^{max}$	Maximum storage capacity of storage type s for product form i	kg
SSC_{si}	Capital cost of establishing storage type s storing product form i	$
USC_{si}	Unit storage cost for product form i at storage type s	$ per kg-day
β	Storage holding period-average number of days worth of stock	days
GW_i^{Stock}	Storage global warming potential form i	g CO_2-equiv per kg of H_2
RS_s	Risk level in storage facility s	units
Transportation data		
$AD_{gg'}$	Average delivery distance between grids g and g' by transportation mode l	km per trip
$RR_{gg'}$	Road risk between grids g and g'	units

(*continued on next page*)

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Table A.2 (*continued*)

W_l	Weight of transportation mode *l*	tons
DW_l	Driver wage of transportation mode *l*	$ per hour
FE_l	Fuel economy of transportation mode *l*	km per litre
FP_l	Fuel price of transportation mode *l*	$ per litre
GE_l	General expenses of transportation mode *l*	$ per day
LUT_l	Load and unload time of product for transportation mode *l*	hours per trip
ME_l	Maintenance expenses of transportation mode *l*	$ per km
SP_l	Average speed of transportation mode *l*	km per hour
TMA_l	Availability of transportation mode *l*	hours per day
GW_l^{Trans}	Global warming potential of transportation mode *l*	g CO_2 per tonne-km
RT_l	Risk level of transportation mode *l*	
$TCap_{il}$	Capacity of transportation mode *l* transporting product form *i*	kg per trip
$Qmin_{il}$	Minimum flow rate of product form *i* by transportation mode *l*	kg per day
$Qmax_{il}$	Maximum flow rate of product form *i* by transportation mode *l*	kg per day
TMC_{il}	Cost of establishing transportation mode *l* transporting product form *i*	$

Table A.3 – Variables.

Continuous variables		
DL_{ig}	Demand for product form *i* in grid *g* satisfied by local production	kg per day
DI_{ig}	Imported demand of product form *i* to grid *g*	kg per day
PR_{pig}	Production rate of product form *i* produced by plant type *p* in grid *g*	kg per day
PT_{ig}	Total production rate of product *i* in grid *g*	kg per day
PGW^{Prod}	Total daily global warming potential in the production facilities *p*	g CO_2-equiv per day
TPRisk	Total risk index for production activity *p*	
ST_{ig}	Total average inventory of product form *i* in grid *g*	kg
SGW^{Stock}	Total daily global warming potential in the storage technology *s*	g CO_2-equiv per day
TSRisk	Total risk index for storage activity *s*	
$Q_{ilgg'}$	Flow rate of product form *i* by transportation mode *l* between grids *g* and *g′*	kg per day
FC	Fuel cost	$ per day
GC	General cost	$ per day
LC	Labour cost	$ per day
MC	Maintenance cost	$ per day
$V_{ilgg'}$	Artificial variable with values between 0 and 1	
TGW^{Trans}	Total daily global warming potential in the transportation mode *l*	g CO_2-equiv per day
TTRisk	Total risk index for transport activity	
FCC	Facility capital cost	$
FOC	Facility operating cost	$ per day

Table A.3 (*continued*)

TCC	Transportation capital cost	$
TOC	Transportation operating cost	$ per day
GWPTot	Total global warming potential of the network	g CO_2-equiv per day
TotalRisk	Total risk of this configuration	
TDC	Total daily cost of the network	$ per day
Integer variables		
NP_{pig}	Number of plants of type *p* producing product form *i* in grid *g*	
NS_{sig}	Number of storage facilities of type *s* for product form *i* in grid *g*	
$NTU_{ilgg'}$	Number of transport units between *g* and *g′*	
Binary variables		
$X_{ilgg'}$	1 when the product form *i* is to be transported from grids *g* to *g*.	
Y_{ig}	1 if product form *i* is to be exported from grid *g* or 0 otherwise	
Z_{ig}	1 if product form *i* is to be imported into grid *g* or 0 otherwise	

A.4 – Almansoori and Shah [17] mathematical model

1. Demand constraints

$$D^L_{ig} \le P^T_{ig} \quad \forall i, g \tag{A.4.1}$$

$$D^I_{ig} = \sum_{l,g'} Q_{ilg'g} \quad \forall i, g;\ g \ne g' \tag{A.4.2}$$

$$D^T_{ig} = D^L_{ig} + D^I_{ig} \quad \forall i, g \tag{A.4.3}$$

2. Production facilities constraints

$$P^T_{ig} = \sum_{l,g'} \left(Q_{ilgg'} - Q_{ilg'g} \right) + D^T_{ig} \quad \forall i, g \tag{A.4.4}$$

$$P^T_{ig} = \sum_{p} PR_{pig} \quad \forall i, g \tag{A.4.5}$$

$$PCap^{min}_{pi} NP_{pig} \le PR_{pig} \le PCap^{max}_{pi} NP_{pig} \quad \forall p, i, g \tag{A.4.6}$$

$$\sum_{p} PCap^{min}_{pi} NP_{pig} \le P^T_{ig} \le \sum_{p} PCap^{max}_{pi} NP_{pig} \quad \forall i, g \tag{A.4.7}$$

3. Transportation constraints

$$Q^{min}_{il} X_{ilgg'} \le Q_{ilgg'} \le Q^{max}_{il} X_{ilgg'} \quad \forall i, l, g, g';\ g \ne g' \tag{A.4.8}$$

$$X_{ilgg'} + X_{ilg'g} \le 1 \quad \forall i, l, g, g';\ g \ne g' \tag{A.4.9}$$

$$Y_{igt} \ge X_{ilgg'} \quad \forall i, l, g, g';\ g \ne g' \tag{A.4.10}$$

$$Z_{ig} \ge X_{ilg'g} \quad \forall i, l, g, g';\ g \ne g' \tag{A.4.11}$$

$$Y_{ig} + Z_{ig} \le 1 \quad \forall i, g \tag{A.4.12}$$

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4. Storage facility constraints

$$S^T_{ig} = \beta D^T_{ig} \quad \forall i, g \tag{A.4.13}$$

$$\sum_s SCap^{min}_{si} NS_{sig} \leq S^T_{ig} \leq \sum_s SCap^{miax}_{si} NS_{sig} \quad \forall i, g \tag{A.4.14}$$

Objective Function elements (for total daily cost)

a) Facility capital cost

$$FCC = \sum_{i,g} \quad \sum_p PCC_{pi} NP_{pig} + \sum_s SCC_{si} NS_{sig} \Big) \tag{A.4.15}$$

b) Transportation capital cost

$$NTUgrid_{ilgg'} = \left(\frac{Q_{ilgg'}}{TMA_l TCap_{il}} \left(\frac{2AD_{gg'}}{SP_l} + LUT_l \right) \right) \tag{A.4.16}$$

$$TCC = \sum_{ilgg'} NTUgrid_{ilgg'} x TMC_{il} \tag{A.4.17}$$

c) Facility operating cost

$$FOC = \sum_{i,g} \quad \sum_p UPC_{pi} PR_{pig} + \sum_s USC_{si} S^T_{ig} \Big) \tag{A.4.18}$$

d) Transportation operating cost

$$FC = \sum_{i,l,g,g'} FP_l \left(\frac{2AD_{gg'} Q_{ilgg'}}{FE_l TCap_{il}} \right) \tag{A.4.19}$$

$$LC = \sum_{i,l,g,g'} DW_l \left(\frac{Q_{ilgg'}}{TCap_{il}} \left(\frac{2AD_{gg'}}{SP_l} + LUT_l \right) \right) \tag{A.4.20}$$

$$MC = \sum_{i,l,g,g'} ME_l \left(\frac{2AD_{gg'} Q_{ilgg'}}{TCap_{il}} \right) \tag{A.4.21}$$

$$GC = \sum_{i,l,g,g'} GE_l \left(\frac{\left(Q_{ilgg'}\right)}{TMA_l TCap_{il}} \left(\frac{2AD_{gg'}}{SP_l} + LUT_l \right) \right) \tag{A.4.22}$$

$$TOC = FC + LC + MC + GC \tag{A.4.23}$$

Appendix B. Supply chain decision database

Table B.1 – Total demand for product form *i* in grid *g* (kg per day).

Grid	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Liquid H_2	102,000	80,000	158,000	198,000	41,000	13,0000	173,000	7000	85,000	316,000	385,000	9000	635,000	902,000
Grid	15	16	17	18	19	20	21	22	23	24	25	26	27	28
Liquid H_2	143,000	24,000	489,000	997,000	500,000	41,000	63,000	624,000	1,000,000	861,000	356,000	63,000	394,000	879,000
Grid	29	30	31	32	33	34	Total (kg per day)							
Liquid H_2	3,000,000	200,000	208,000	252,000	200,000	136,000	**13,395,000**							

Table B.2 – Parameters for hydrogen supply chain components: (a) general data, (b) production, (c) storage, and (d) transportation modes.

(a) General data

α	Network operating period	365 days per year
CCF	Capital change factor -payback period of capital investment	3 years
WFP_g	Weight factor risk population in each grid	Units (see Table 3)

(*continued on next page*)

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Table B.2 (*continued*)

(b) Production plants

Plant type, p	Steam methane reforming	Biomass gasification	Coal gasification	Reference
Minimum production capacity of plant type p for product form i. $PCap_{pi}^{min}$ (t/d)	10	10	10	[17]
Maximum production capacity of plant type p for product form i. $PCap_{pi}^{max}$ (t/d)	480	480	480	[17]
Capital cost of establishing plant type p producing product form i. PCC_{pi} (M$)	535	1412	958	[17]
Unit production cost for product form i produced by plant type p. UPC_{pi} ($ per kg)	1.53	3.08	1.71	[17]
Production global warming potential by plant type p. GW_p^{Prod} (g CO_2-equiv per kg H_2)	10,100	3100	10,540	[25,32,34]
Risk level of the production facility p. RP_p level	III	III	III	[21]

(c) Storage data

Storage type, s	Liquid storage	Ref.
Minimum storage capacity of storage type s for product form i. $SCap_{si}^{min}$ (kg)	10,000	[17]
Maximum storage capacity of storage type s for product form i. $SCap_{si}^{max}$ (kg)	540,000	[17]
Capital cost of establishing storage type s storing product form i. SSC_{si} ($)	122,000,000	[17]
Unit storage cost for product form i at storage type s. USC_{si} ($ per kg per day)	0.005	[17]
Storage holding period − average number of days worth of stock. β (days)	10	[17]
Storage global warming potential form i. GW_i^{Stock} (g CO_2-equiv per kg of H_2)	5241	[33]
Risk level in storage facility s. RS_s (units)	III	[21]

(d) Transportation modes

Transportation mode, l	Tanker truck	Ref.
Transport unit capacity, $TCap_{il}$ (kg/mode)	4082	[17]
Fuel economy between grids, FE_l (km/L)	2.55	[17]
Average speed between grids, SP_l (km/h)	55	[17]
Tanker truck weight, w_l (t)	40	[35]
Mode availability between grids, TMA_l (h/d)	18	[17]
Load/unload time, LUT_l (h)	2	[17]
Driver wage, DW_l ($/h)	23	[17]
Fuel price, FP_l ($/L)	1.16	[17]
Maintenance expenses, ME_l ($/km)	0.0976	[17]
General expenses, GE_l ($/d)	8.22	[17]
Transport mode cost, TMC_{il} ($/mode)	500,000	[17]
Minimum flow rate of product form i, $Qmin_{il}$ (kg/d)	4082	[17]
Maximum flow rate of product form i, $Qmax_{il}$ (t/d)	960	[17]
Global warming potential, $GWTrans_l$ (g CO_2 per tonne-km)	62	[35]
Risk level of transportation mode l, RT_l (level)	III	[21]

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Table B.3 — Delivery distances within and between different grids squares (km per trip).

Grid	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34
1	**65**	108	108	152	206	216	241	344	328	341	415	404	446	482	536	664	587	580	631	730	706	682	682	723	831	791	788	785	821	843	972	899	837	852
2	108	**65**	152	152	197	247	247	352	346	351	459	408	457	492	529	673	597	587	648	746	715	691	691	749	835	802	795	795	827	853	983	909	848	861
3	108	152	**65**	108	162	108	152	248	222	241	323	298	344	389	421	563	487	482	539	637	655	581	580	628	736	743	689	685	723	749	870	796	735	751
4	152	152	108	**65**	54	152	108	216	222	216	282	290	323	349	390	533	457	449	496	596	577	553	552	590	663	663	656	656	688	710	843	769	709	722
5	206	197	162	54	**65**	194	120	228	241	228	291	314	332	361	399	548	471	461	509	609	590	566	565	602	675	677	670	670	701	723	856	783	723	735
6	216	247	108	152	194	**65**	108	170	120	152	241	197	248	305	345	476	400	389	457	551	510	492	484	539	617	606	597	597	629	658	787	713	650	662
7	241	247	152	108	120	108	**65**	108	120	108	174	194	216	241	283	427	351	341	389	488	469	445	444	482	555	556	550	550	580	602	736	662	602	614
8	344	352	248	216	228	170	108	**65**	120	76	76	194	170	170	194	368	292	275	314	415	403	381	381	410	482	502	488	488	511	531	679	605	542	550
9	328	346	222	222	241	120	120	120	**65**	54	162	76	130	194	241	359	283	271	345	435	401	375	366	421	502	489	448	480	514	540	670	596	533	537
10	341	351	241	216	228	152	108	76	54	**65**	108	54	108	152	194	323	247	241	305	399	365	343	341	389	466	451	444	444	482	508	629	555	497	511
11	415	459	323	282	291	241	174	76	162	108	**65**	222	152	108	130	323	247	216	248	344	361	341	323	341	411	451	444	431	444	460	629	555	485	488
12	404	408	298	290	314	197	194	194	76	54	222	**65**	162	228	278	390	314	302	377	467	423	406	406	453	533	507	500	500	542	571	686	612	552	568
13	446	457	344	323	332	248	216	170	130	108	152	162	**65**	108	162	229	152	152	241	323	271	247	247	305	390	359	351	351	389	421	540	466	404	410
14	482	492	389	349	361	305	241	170	194	152	108	228	108	**65**	54	229	152	108	152	248	271	241	216	241	361	349	341	323	341	361	522	448	377	381
15	536	529	421	390	399	345	283	194	241	194	130	278	162	54	**65**	269	194	120	120	224	305	269	222	222	343	381	361	328	328	341	535	461	381	377
16	664	673	563	533	548	476	427	368	359	323	323	390	229	229	269	**65**	76	170	275	323	54	76	170	275	381	130	170	229	314	361	389	315	269	305
17	587	597	487	457	471	400	351	292	283	247	247	314	152	152	194	76	**65**	108	216	276	120	108	152	241	341	197	216	241	305	345	416	343	290	314
18	580	587	482	449	461	389	341	275	271	241	216	302	152	108	120	170	108	**65**	108	174	194	152	108	152	241	269	241	216	241	269	416	343	269	275
19	631	648	539	496	509	457	389	314	345	305	248	377	241	152	120	275	216	108	**65**	108	290	241	152	108	174	361	305	241	216	224	464	389	290	275
20	730	746	637	596	609	551	488	415	435	399	344	467	323	248	224	323	276	174	108	**65**	328	275	170	76	76	392	314	229	170	162	464	381	269	241
21	706	715	655	577	590	510	469	403	401	365	361	423	271	271	305	54	120	194	290	328	**65**	54	162	269	377	76	120	194	290	341	347	273	229	269
22	682	691	581	553	566	492	445	381	375	343	341	406	247	241	269	76	108	152	241	275	54	**65**	108	216	323	120	108	152	241	290	315	241	194	229
23	682	691	580	552	565	484	444	381	366	341	323	406	247	216	222	170	152	108	152	170	162	108	**65**	108	216	222	152	108	152	194	315	241	162	170
24	723	749	628	590	602	539	482	410	421	389	341	453	305	241	222	275	241	152	108	76	269	216	108	**65**	108	328	241	152	108	120	389	305	194	170
25	831	835	736	663	675	617	555	482	502	466	411	533	390	361	343	381	341	241	174	76	377	323	216	108	**65**	434	341	241	152	130	484	415	269	229
26	791	802	743	663	677	606	556	502	489	451	451	507	359	349	381	130	197	269	361	392	76	120	222	328	434	**65**	120	222	328	381	365	291	247	290
27	788	795	689	656	670	597	550	488	448	444	444	500	351	341	361	170	216	241	305	314	120	108	152	241	341	120	**65**	108	216	269	248	174	130	174
28	785	795	685	656	670	597	550	488	480	444	431	500	351	323	328	229	241	216	241	229	194	152	108	152	241	222	108	**65**	108	162	241	174	54	76
29	821	827	723	688	701	629	580	511	514	482	444	542	389	341	328	314	305	241	216	170	290	241	152	108	152	328	216	108	**65**	54	341	276	120	76
30	843	853	749	710	723	658	602	531	540	508	460	571	421	361	341	361	345	269	224	162	341	290	194	120	130	381	269	162	54	**65**	392	329	170	120
31	972	983	870	843	856	787	736	679	670	629	629	686	540	522	535	389	416	416	464	464	347	315	315	389	484	365	248	241	341	392	**65**	108	222	275
32	899	909	796	769	783	713	662	605	596	555	555	612	466	448	461	315	343	343	389	381	273	241	241	305	415	291	174	174	276	329	108	**65**	162	216
33	837	848	735	709	723	650	602	542	533	497	485	552	404	377	381	269	290	269	290	269	229	194	162	194	269	247	130	54	120	170	222	162	**65**	54
34	852	861	751	722	735	662	614	550	537	511	488	568	410	381	377	305	314	275	275	241	269	229	170	170	229	290	174	76	76	120	275	216	54	**65**

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Table B.4 – Total relative road risk matrix (units).

Grid	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34
1	0	3	4	6	7	6	8	9	7	9	11	8	13	15	17	16	15	18	20	22	19	18	21	23	25	20	20	24	27	29	24	22	26	28
2	3	0	5	3	4	7	5	6	8	7	9	9	10	12	14	16	15	15	17	21	19	18	21	24	26	20	20	24	27	29	30	28	26	28
3	4	5	0	4	5	4	6	7	5	8	10	6	11	13	15	16	15	16	18	24	19	18	21	22	24	20	20	24	25	27	30	28	26	26
4	6	3	4	0	3	6	4	5	7	6	8	8	9	12	14	14	13	15	17	23	17	16	18	20	22	19	18	21	23	25	27	25	23	24
5	7	4	5	3	0	7	5	6	9	7	9	10	10	12	14	18	17	15	17	22	21	20	18	21	23	23	21	21	24	26	27	25	23	25
6	6	7	4	6	7	0	4	5	3	6	8	4	9	11	13	12	11	14	16	22	15	14	17	20	22	16	16	20	23	25	19	18	22	24
7	8	5	6	4	5	4	0	3	5	4	6	6	7	10	12	10	9	13	14	20	13	12	16	19	21	15	14	19	22	24	24	23	24	23
8	9	6	7	5	6	5	3	0	6	5	3	7	8	6	8	11	10	9	11	17	14	13	12	15	17	16	15	15	18	20	21	19	17	19
9	7	8	5	7	9	3	5	6	0	3	5	2	6	8	10	9	8	11	13	19	12	11	14	17	19	13	13	17	20	22	23	21	19	20
10	9	7	8	6	7	6	4	5	3	0	4	5	5	8	10	8	7	11	13	19	11	10	14	17	19	13	12	17	20	22	22	21	19	20
11	11	9	10	8	9	8	6	3	5	4	0	6	8	5	7	11	10	8	10	16	15	14	11	14	16	17	16	14	17	19	20	18	16	18
12	8	9	6	8	10	4	6	7	2	5	6	0	7	10	12	10	9	13	15	21	20	19	16	19	21	22	21	19	22	24	25	23	21	23
13	13	10	11	9	10	9	7	8	6	5	8	7	0	6	8	6	5	9	11	17	16	15	12	15	17	18	17	15	18	20	21	19	17	19
14	15	12	13	12	12	11	10	6	8	8	5	10	6	0	5	9	8	6	8	14	13	12	9	12	14	15	14	12	15	17	18	16	14	16
15	17	14	15	14	14	13	12	8	10	10	7	12	8	5	0	11	10	8	4	10	15	14	11	7	9	17	16	14	10	12	20	18	16	11
16	16	16	16	14	18	12	10	11	9	8	11	10	6	9	11	0	3	6	8	14	7	6	9	12	14	9	8	11	14	16	15	13	13	14
17	15	15	15	13	17	11	9	10	8	7	10	9	5	8	10	3	0	5	7	13	6	5	8	11	13	8	7	10	13	15	14	12	12	13
18	18	15	16	15	15	14	13	9	11	11	8	13	9	6	8	6	5	0	5	11	9	8	6	9	11	11	10	9	12	14	15	13	13	14
19	20	17	18	17	17	16	14	11	13	13	10	15	11	8	4	8	7	5	0	8	11	10	8	5	7	13	12	11	8	10	17	15	13	14
20	22	21	24	23	22	22	20	17	19	19	16	21	17	14	10	14	13	11	8	0	13	12	9	6	3	14	14	12	9	5	18	16	14	15
21	19	19	19	17	21	15	13	14	12	11	15	20	16	13	15	7	6	9	11	13	0	4	7	10	12	2	4	7	10	12	11	9	9	10
22	18	18	18	16	20	14	12	13	11	10	14	19	15	12	14	6	5	8	10	12	4	0	6	9	11	6	5	9	12	14	15	13	11	12
23	21	21	21	18	18	17	16	12	14	14	11	16	12	9	11	9	8	6	8	9	7	6	0	6	8	9	8	6	9	11	12	10	8	9
24	23	24	22	20	21	20	19	15	17	17	14	19	15	12	7	12	11	9	5	6	10	9	6	0	5	12	11	9	6	8	15	13	11	7
25	25	26	24	22	23	22	21	17	19	19	16	21	17	14	9	14	13	11	7	3	12	11	8	5	0	14	13	11	8	10	17	15	13	9
26	20	20	20	19	23	16	15	16	13	13	17	22	18	15	17	9	8	11	13	14	2	6	9	12	14	0	3	6	9	11	10	8	8	9
27	20	20	20	18	21	16	14	15	13	12	16	21	17	14	16	8	7	10	12	14	4	5	8	11	13	3	0	5	8	10	9	7	7	8
28	24	24	24	21	21	20	19	15	17	17	14	19	15	12	14	11	10	9	11	12	7	9	6	9	11	6	5	0	6	8	9	7	5	6
29	27	27	25	23	24	23	22	18	20	20	17	22	18	15	10	14	13	12	8	9	10	12	9	6	8	9	8	6	0	5	12	10	8	4
30	29	29	27	25	26	25	24	20	22	22	19	24	20	17	12	16	15	14	10	5	12	14	11	8	10	11	10	8	5	0	14	12	10	6
31	24	30	30	27	27	19	24	21	23	22	20	25	21	18	20	15	14	15	17	18	11	15	12	15	17	10	9	9	12	14	0	4	6	7
32	22	28	28	25	25	18	23	19	21	21	18	23	19	16	18	13	12	13	15	16	9	13	10	13	15	8	7	7	10	12	4	0	4	5
33	26	26	26	23	23	22	24	17	19	19	16	21	17	14	16	13	12	13	13	14	9	11	8	11	13	8	7	5	8	10	6	4	0	3
34	28	28	26	24	25	24	23	19	21	20	18	23	19	16	11	14	13	14	14	15	10	12	9	7	9	9	8	6	4	6	7	5	3	0
Total	531	526	515	469	514	434	414	372	386	374	377	462	402	373	390	367	335	360	385	492	391	389	378	428	487	421	400	420	472	530	565	507	475	487

Table B.5 – Level risk according to harmfulness for people, the environment and facilities for hydrogen activities [21].

Harmfulness for	Level II	Level III	Level IV
People	Medical treatment and lost time injury	Permanent disability	Several fatalities
Environment	Damage of short duration (<1 month)	Time for restitution of ecological resource (<1 year)	Time for restitution of ecological resource (1–3 years)
Facilities	Minor structural damage and minor influence on operations.	Considerable structural damage and operation interrupted for weeks	Loss of main part of system and operation interrupted for months.
Weighted scoring method	3	5	7

Table B.6 – Example of external effect factors gained during transportation from grid 1 to 33.

		From grid 1 to 33		
Grid	Size	Grid safety level	Weight factor of adjacency level	Total
1	Med	2	1	2
2	Small	1	0.5	0.5
3	Med	2	0.5	1
4	Med	2	1	2
5	Small	1		0
6	Med	2		0
7	Med	2	1	2
8	Small	1		0
9	Small	1		0
10	Med	2	1	2
11	Med	2		0
12	Small	1		0
13	Large	3	1	3
14	Large	3		0
15	Med	2		0
16	Small	1		0
17	Med	2	1	2
18	Large	3	0.5	1.5
19	Med	2		0
20	Small	1		0
21	Small	1		0
22	Large	3	0.5	1.5
23	Large	3	1	3
24	Large	3		0
25	Med	2		0
26	Small	1		0
27	Med	2		0
28	Large	3	1	3
29	Large	3		0
30	Med	2		0
31	Med	2		0
32	Med	2		0
33	Med	2	1	2
34	Small	1		0
Total				25.5

Appendix C. Detailed results

Table C.1 – Flow rate of liquid hydrogen via tanker truck for cases 1–4.

From grid	To grid	Flow rate, $Q_{ilgg'}$ (kg d^{-1})
(a) Case 1. Mono-objective optimization. Min TDC.		
3	1	102,130
3	2	80,020
3	4	12,396
3	6	123,203
7	4	185,544
7	5	41,060
7	6	6297
7	8	7370
7	9	67,059
10	9	18,221
10	12	9480
10	13	136,359
11	13	9761
11	15	87,377
14	13	8910
14	15	48,850
22	16	24,450
22	17	8520
22	18	36,640
22	21	63,170
22	23	87,490
22	26	62,810
22	33	14,101
24	15	6693
24	19	11,453
24	30	80,824
25	19	5977
25	20	40,610
25	30	74,212
27	33	86,270
28	33	66,036
28	34	15,424
29	30	32,924
29	34	120,506
32	31	207,720
32	33	18,623
Total		2,008,490
(b) Cases 2–4. Lexicographic/Multi-objective optimizations.		
9	12	9480
11	8	7370
16	17	8520
Total		25,370

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Table C.2 – Summary of results for cases 1–4.

Case 1					*Cases 2, 3 and 4*		
Variable	DL_{ig} (kg d^{-1})	DI_{ig} (kg d^{-1})	PT_{ig} (kg d^{-1})	ST_{ig} (t)[a]	DL_{ig} (kg d^{-1})	DI_{ig} (kg d^{-1})	PT_{ig} (kg d^{-1})
G.1	–	102,130	–	1021.3	102,130	–	102,130
G.2	–	80,020	–	800.2	80,020	–	80,020
G.3	157,930	–	475,679	1579.3	157,930	–	157,930
G.4	–	197,940	–	1979.4	197,940	–	197,940
G.5	–	41,060	–	410.6	41,060	–	41,060
G.6	–	129,500	–	1295	129,500	–	129,500
G.7	172,670	–	480,000	1726.7	172,670	–	172,670
G.8	–	7370	–	73.7	–	7370	
G.9	–	85,280	–	852.8	85,280	–	94,760
G.10	315,940	–	480,000	3159.4	315,940	–	315,940
G.11	382,810	–	479,948	3828.1	382,810	–	390,180
G.12	–	9480		94.8	–	9480	
G.13	480,000	155,030	480,000	6350.3	635,030	–	635,030
G.14	902,240	–	960,000	9022.4	902,240	–	902,240
G.15	–	142,920	–	1429.2	142,920	–	142,920
G.16	–	24,450	–	244.5	24,450	–	32,970
G.17	480,000	8520	480,000	4885.2	480,000	8520	480,000
G.18	960,000	36,640	960,000	9966.4	996,640	–	996,640
G.19	480,000	17,430	480,000	4974.3	497,430	–	497,430
G.20	–	40,610	–	406.1	40,610	–	40,610
G.21	–	63,170	–	631.7	63,170	–	63,170
G.22	623,950	–	921,131	6239.5	623,950	–	623,950
G.23	960,000	87,490	960,000	10,474.9	1,047,490	–	1,047,490
G.24	861,030	–	960,000	8610.3	861,030	–	861,030
G.25	356,500	–	477,299	3565	356,500	–	356,500
G.26	–	62,810	–	628.1	62,810	–	62,810
G.27	393,730	–	480,000	3937.3	393,730	–	393,730
G.28	878,540	–	960,000	8785.4	878,540	–	878,540
G.29	2,726,570	–	2,880,000	27,265.7	2,726,570	–	2,726,570
G.30	–	187,960	–	1879.6	187,960	–	187,960
G.31	–	207,720	–	2077.2	207,720	–	207,720
G.32	252,230		478,573	2522.3	252,230	–	252,230
G.33	–	185,030	–	1850.3	185,030	–	185,030
G.34	–	135,930	–	1359.3	135,930	–	135,930

a ST_{ig} is only given for network case 1 since networks 2, 3 and 4 have the same values.

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Table C.3 – Comparison between results in TOPSIS and M-TOPSIS.

Alternatives	Criteria value			TOPSIS		M-TOPSIS	
	Total risk (units)	TDC (M$ per day)	Total GWP (thousand t CO_2-equiv CO_2-equiv per day)	Ratio TOPSIS	Rank	Ratio M-TOPSIS	Rank
1	5970	132.05	111.85	0.4539	25	0.0462	24
2	5970	126.86	113.59	0.4363	22	0.0494	21
3	5970	124.07	115.33	0.4272	14	0.0513	16
4	5970	122.09	117.07	0.4212	11	0.0525	13
5	5970	120.10	118.81	0.4148	8	0.0540	11
6	5970	118.11	120.55	0.4081	7	0.0555	8
7	5970	116.93	122.29	0.4053	6	0.0562	6
8	5970	109.01	132.74	0.0.3838	3	0.0617	3
9	5970	103.49	143.19	0.3786	1	0.0632	2
10	5970	97.97	153.63	0.3790	2	0.0634	1
11	5970	93.26	164.08	0.3896	4	0.0.0608	4
12	5970	88.54	174.52	0.4039	5	0.0568	5
13	5970	83.83	184.97	0.4197	9	0.0522	14
14	5970	79.11	195.41	0.4350	20	0.0479	23
15	5970	73.65	205.60	0.4459	23	0.0460	26
16	8132	110.89	113.59	0.4321	19	0.0492	22
17	8132	109.70	115.33	0.4297	16	0.0501	20
18	8132	109.01	117.07	0.4299	17	0.0503	19
19	8132	108.30	118.81	0.4301	18	0.0505	18
20	8132	107.11	120.55	0.4278	15	0.0514	15
21	8132	105.42	122.29	0.4227	12	0.0531	12
22	8132	100.22	132.74	0.4210	10	0.0555	9
23	8132	95.50	143.19	0.4262	13	0.0558	7
24	8132	90.79	153.63	0.4356	21	0.0544	10
25	8132	86.57	164.08	0.4505	24	0.0506	17
26	8132	81.36	174.52	0.4609	26	0.0460	25
27	8132	76.68	184.89	0.4732	27	0.0402	27
28	8132	71.92	195.41	0.4837	28	0.0347	28
29	8132	67.05	205.75	0.4913	29	0.0318	29
30	10,292.5	108.88	113.59	0.5104	30	0.0262	35
31	10,292.5	108.02	115.33	0.5114	32	0.0260	36
32	10,292.5	106.81	117.07	0.5111	31	0.0264	32
33	10,292.5	106.47	118.81	0.5142	34	0.0258	37
34	10,292.5	105.26	120.55	0.5139	33	0.0262	33
35	10,292.5	104.91	122.29	0.5170	35	0.0258	38
36	10,292.5	99.87	132.74	0.5247	36	0.0266	31
37	10,292.5	95.13	143.19	0.5340	37	0.0268	30
38	10,292.5	89.93	153.63	0.5402	38	0.0262	34
39	10,292.5	85.29	164.08	0.5475	40	0.0236	39
40	10,292.5	80.51	174.47	0.5517	43	0.0197	41
41	10,292.5	75.43	184.40	0.5510	41	0.0159	42
42	10,292.5	70.72	194.70	0.5513	42	0.0140	43
43	10,292.5	64.57	205.86	0.5461	39	0.0201	40

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Nomenclature

Indices

g: grid squares and g': grid squares such that $g' \neq g$
i: product physical form
l: type of transportation modes
p: plant type with different production technologies
s: storage facility type with different storage technologies

Parameters

General data

DT_{ig}: total demand for product form i in grid g, kg per day
α: network operating period, days per year
CCF: capital change factor – payback period of capital investment, years
WFP_g: weight factor risk population in each grid, units

Production data

$PCap_{pi}^{min}$: minimum production capacity of plant type p for product form i, kg per day
$PCap_{pi}^{max}$: maximum production capacity of plant type p for product form i, kg per day
PCC_{pi}: capital cost of establishing plant type p producing product form i, \$

UPC^{pi}: unit production cost for product form i produced by plant type p, \$ per kg

GW_p^{Prod}: production global warming potential by plant type p, g CO_2-equiv per kg of H_2

RP_p: risk level of the production facility p, units

Storage data

$SCap_{si}^{min}$: minimum storage capacity of storage type s for product form i, kg

$SCap_{si}^{max}$: maximum storage capacity of storage type s for product form i, kg

SSC_{si}: capital cost of establishing storage type s storing product form i, \$

USC_{si}: unit storage cost for product form i at storage type s, \$ per kg-day

β: storage holding period-average number of days worth of stock, days

GW_i^{Stock}: storage global warming potential form i, g CO_2-equiv per kg of H_2

RS_s: risk level in storage facility s, units

Transportation data

$AD_{gg'}$: average delivery distance between grids g and g' by transportation mode l, km per trip

$RR_{gg'}$: road risk between grids g and g', units

Bg: adjacency level weight factor of a region g in which the route is located, units

RL_g: risk level of the grid g, units

W_l: weight of transportation mode l, tons

DW_l: driver wage of transportation mode l, \$ per hour

FE_l: fuel economy of transportation mode l, km per litre

FP_l: fuel price of transportation mode l, \$ per litre

GE_l: general expenses of transportation mode l, \$ per day

LUT_l: load and unload time of product for transportation mode l, hours per trip

ME_l: maintenance expenses of transportation mode l, \$ per km

SP_l: average speed of transportation mode l, km per hour

TMA_l: availability of transportation mode l, hours per day

GW_l^{Trans}: global warming potential of transportation mode l, g CO_2 per tonne-km

RT_l: risk level of transportation mode l, units

$TCap_{il}$: capacity of transportation mode l transporting product form i, kg per trip

$Qmin_{il}$: minimum flow rate of product form i by transportation mode l, kg per day

$Qmax_{il}$: maximum flow rate of product form i by transportation mode l, kg per day

TMC_{il}: cost of establishing transportation mode l transporting product form I, \$

Variables

Continuous variables

DL_{ig}: demand for product form i in grid g satisfied by local production, kg per day

DI_{ig}: imported demand of product form i to grid g, kg per day

PR_{pig}: production rate of product form i produced by plant type p in grid g, kg per day

PT_{ig}: total production rate of product i in grid g, kg per day

PGW^{Prod}: total daily global warming potential in the production facilities p, g CO_2-equiv per day

TPRisk: total risk index for production activity p, units

ST_{ig}: total average inventory of product form i in grid g, kg

SGW^{Stock}: total daily global warming potential in the storage technology s, g CO_2-equiv per day

TSRisk: total risk index for storage activity s, units

$Q_{ilgg'}$: flow rate of product form i by transportation mode l between grids g and g', kg per day

FC: fuel cost, \$ per day

GC: general cost, \$ per day

LC: labour cost, \$ per day

MC: maintenance cost, \$ per day

$V_{ilgg'}$: artificial variable with values between 0 and 1

TGW^{Trans}: total daily global warming potential in the transportation mode l, g CO_2-equiv per day

TTRisk: total risk index for transport activity, units

FCC: facility capital cost, \$

FOC: facility operating cost, \$ per day

TCC: transportation capital cost, \$

TOC: transportation operating cost, \$ per day

GWPTot: total global warming potential of the network, g CO_2-equiv per day

TotalRisk: total risk of this configuration, units

TDC: total daily cost of the network, \$ per day

Integer variables

NP_{pig}: number of plants of type p producing product form i in grid g

NS_{sig}: number of storage facilities of type s for product form i in grid g

$NTU_{ilgg'}$: number of transport units between g and g'

Binary variables

$X_{ilgg'}$: 1 when the product form i is to be transported from grids g to g'.

Y_{ig}: 1 if product form i is to be exported from grid g or 0 otherwise

Z_{ig}: 1 if product form i is to be imported into grid g or 0 otherwise

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