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# Design of Experiments for Sensitivity Analysis of a Hydrogen Supply Chain Design Model

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**Abstract**
Hydrogen is one of the most promising energy carriers in the quest for a more sustainable energy mix. In this paper, a model of the hydrogen supply chain (HSC) based on energy sources, production, storage, transportation, and market has been developed through a MILP formulation (Mixed Integer Linear Programming). Previous studies have shown that the start-up of the HSC deployment may be strongly penalized from an economic point of view. The objective of this work is to perform a sensitivity analysis to identify the major parameters (factors) and their interaction affecting an economic criterion, i.e., the total daily cost (TDC) (response), encompassing capital and operational expenditures. An adapted methodology for this SA is the design of experiments through the Factorial Design and Response Surface methods. Six key parameters are chosen (demand, capital change factor (CCF), storage and production capital costs (SCC, PCC), learning rate (LR), and unit production cost (UPC)). The demand is the factor that is by far the most significant parameter that strongly conditions the TDC optimization criterion, the second most significant parameter being the capital change factor. To a lesser extent, the other influencing factors are PCC and LR. The main interactions are found between demand, CCF, UPC, and SCC. The discussion has also shown that the calculation of UPC has to be improved taking into account the contribution of the fixed, electricity, and feedstock costs instead of being considered as a fixed parameter only depending on the size of the production unit. As any change that could occur relative to demand or CCF could strongly affect the response variable, more effort is also needed to find the more consistent way to model demand uncertainty in HSC design, especially since a long horizon time is considered for hydrogen deployment.

**Keywords** Hydrogen supply chain · Sensitivity analysis · Design of experiments

## Introduction

Hydrogen is one of the most promising energy carriers in the quest for a more sustainable energy mix to be used in different applications such as stationary fuel cell systems and electro-mobility applications. Different ways to produce, store, and distribute hydrogen already exist for chemistry applications but, currently, hydrogen is mostly obtained from fossil fuels and hydrogen is generally used for on-site applications. The environmental impacts of hydrogen production, in particular Global Warming Potential, depend mainly on the sources and processes through which hydrogen is derived. A big challenge is then to assess if hydrogen produced from renewable energy sources can turn out to be competitive compared to current fuels and to deploy an infrastructure of hydrogen supply chains (HSC) for new applications. The HSC for the mobility market with $H_2$ as fuel is defined as a system of activities from suppliers to customers. These activities encompass energy source choice, production, storage, transportation, and dispensation of hydrogen to refueling stations (see Fig. 1). Hydrogen can be produced either centrally (similar to existing gasoline supply chains) or distributed at forecourt refueling stations as small scale units that can produce $H_2$ close to the use point in small quantities.

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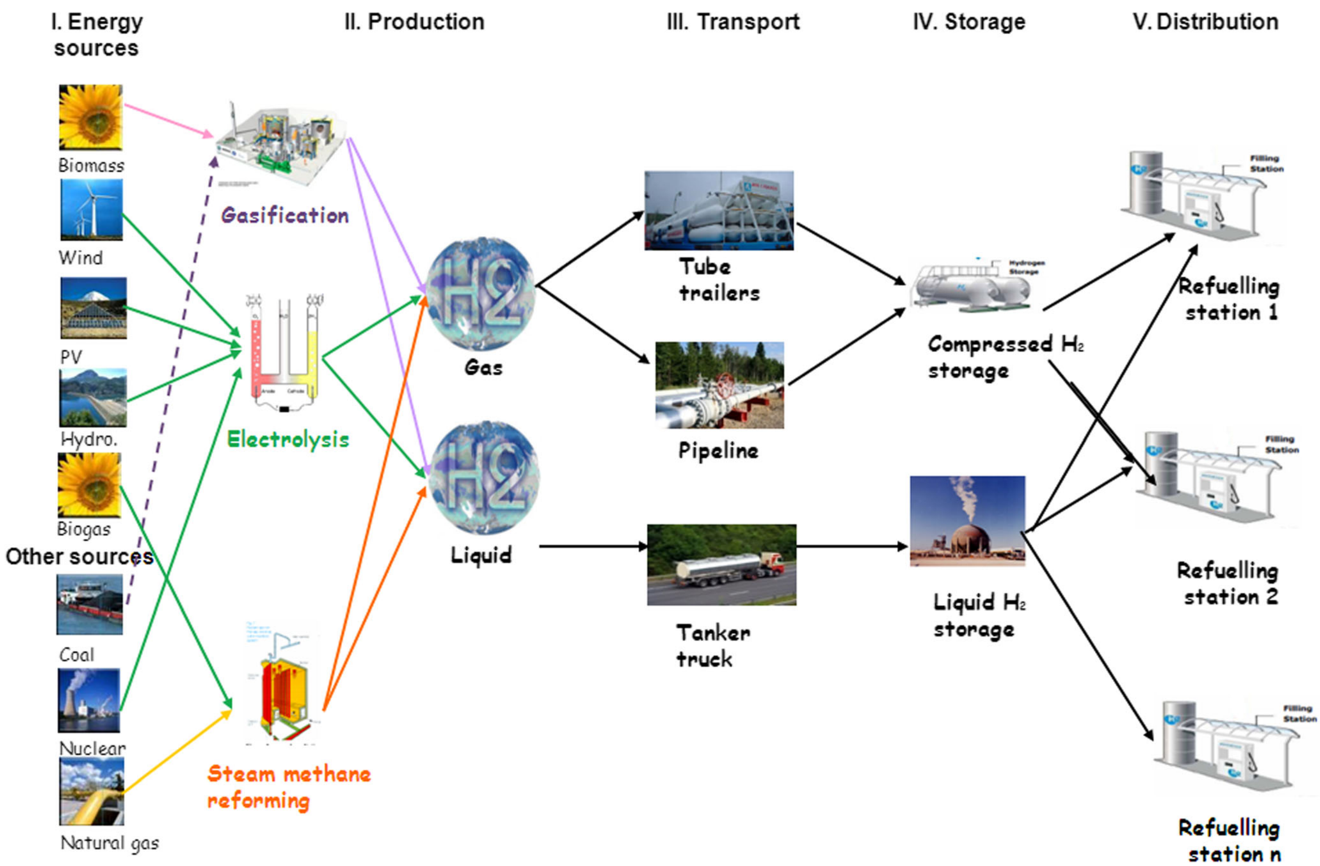


**Fig. 1** HSC example for the Midi Pyrénées region (De León Almaraz et al. 2014)

HSC design can be performed by using optimization and/or geographical simulation tools. The most used approach found in the literature is mathematical programming for optimizing the HSC and representative models can be found in several publications (e.g., Almansoori and Shah 2006; Guillén Gosálbez et al. 2010; Hugo et al. 2005; Kim et al. 2008; Sabio et al. 2010). The formulation is defined for long horizon time period and can be established through multi-period formulation. These works optimize one or more objective functions to find the best HSC design normally prioritizing cost minimization. One of the most referenced work in this topic is that of Almansoori and Shah (2006) which presented a general formulation with a wide database where the total daily cost (TDC) is optimized. The TDC has also been used in works such as Almansoori and Shah (2009, 2012); Kim et al. (2008); and Kim and Moon (2008). Other alternatives to deal with the financial metrics are the net present value (Hugo et al. 2005), investment cost (Ingason et al. 2008; Kamarudin et al. 2009), total discounted cost (Guillén Gosálbez et al. 2010; Sabio et al. 2010); more sophisticated options to evaluate the economic performance of the HSC can be found in (Guillén et al. 2007). The TDC function has also been considered in our previous works (De-León Almaraz et al. 2013, 2014, 2015) since it has the advantage of accounting all the costs incurred in the supply chain excepting the particular interest of one of the stakeholders involved in the value chain. It has been used as one of the objective functions in a multi-objective optimization framework with environmental impact and safety risk as additional criteria to be optimized in mono- and multi-period models and solved using the ε-constraint method at both regional and national scales so that the operability and usefulness of the different scales at a strategic level can be analyzed.

In this work, a deep analysis of the HSC model that optimizes the TDC is performed to identify the main model parameters through a sensitivity analysis (SA) and the subsequent potential improvements in the formulation. A large set of data (parameters) is involved in the mathematical model of the HSC problem. Models for complex systems, such as the HSC one, are often built with more parameters than can be identified by available real data and the parameters of the models use estimated values based on the prospective scenarios. Under these conditions, uncertainty plays a major role and the lack of precise information as well as the use of uncertain forecast proposed for a long time horizon (i.e., outlook for 2050), make the development of a SA mandatory.

## Sensitivity Analysis Concepts and Methods

The SA method is a commonly used approach for identifying important parameters that dominate model behaviors (Gan et al. 2014) and is recommended to evaluate the robustness of the assessment (and thus of the final decision) with respect to uncertain model inputs or assumptions. SA can be applied to learn not only about models but also about systems to identify the critical values of the system drivers that induce threshold effects in the decision objectives (Pianosi et al. 2016). The SA can be implemented from different fields' perspectives, e.g., the operational research uses post-optimal analysis for local sensitivity in linear problems, the economics field uses scenario analysis and statistics have developed a wide number of sophisticated tools for SA. Some of the tools used in the previous fields have been applied to supply chain design problems. Typical questions addressed by SA are as follows (Pianosi et al. 2016):

- What input factors cause the largest variation in the output?
- Is there any factor whose variability has a negligible effect on the output?
- Is there any interaction that amplifies or dampens the variability induced by individual factors?

A vast variety of SA techniques, tools, and software exists and the selection of the right one is not straightforward. They can be evaluated by their effectiveness, efficiency, and consistency in the solution of a given problem. Unfortunately, between heuristics, graphical tools, design of experiments, Monte Carlo techniques, statistical learning methods, etc., beginners and non-specialist users can be found quickly lost on the choice of the most suitable methods for their problem (Iooss and Lemaître 2015). The type of approach, level of complexity, and purposes of SA vary quite significantly depending on the modeling domain and the specific application aims. It therefore guides the choice of the appropriate SA method since different methods are better suited to address different questions. The choice of the method can be also driven by other specific features of the problem at hand, like the linearity of the input-output relationship, the statistical characteristics of the output distribution (e.g., its skew), which are handled more or less effectively by different methods (Pianosi et al. 2016). Four main purposes of the SA are identified in the literature: screening, ranking, mapping, and identification of interactions between input factors. Screening is the process to derive a shortlist with the most important factors. Ranking generates the ranking of the input factors according to their contribution to the output factor. Mapping aims to determine the region of the input variability space.

An input factor is any element that can be changed before model execution. The output factor or response in the case of mathematical modeling can be the objective functions which are optimized. In order to identify the type of SA, it is necessary to distinguish some of its main concepts:

- *Qualitative and quantitative SA*: qualitative methods provide a heuristic score to intuitively represent the relative sensitivity of parameters by visual inspection of model predictions (e.g., tornado plots and scatter plots). In quantitative SA, each input factor is associated with a quantitative evaluation of its relative influence, normally through a set of sensitivity indices on the total variance of model output (Gan et al. 2014; Pianosi et al. 2016; Saltelli et al. 2009; Yang et al. 2014)
- *Local* vs *Global SA*: depending on whether output variability is obtained by varying the inputs around a reference (nominal) value, or across their entire feasible space, SA is either referred to as local or global. Local SA (LSA) applications typically consider model parameters as varying inputs, and aim at assessing how their uncertainty impacts model performance, i.e., how model performance changes when moving away from some optimal or reference parameter set. Global SA (GSA) considers variations within the entire space of variability of the input factors. The GSA does not require the user to specify a nominal value $x$ for the input factors but it still requires specifying the input variability space (Pianosi et al. 2016).
- *One At a Time* vs. *All At a Time SA*: another distinction that is often made lies between One-[factor]-At-a-Time (OAT) and All-[factors]-At-a-Time' (AAT) methods. In OAT test, some factors are fixed OAT while re-estimating the model with the remaining factors. In AAT methods, output variations are induced by varying all the input factors simultaneously, and therefore, the sensitivity to each factor considers the direct influence of that factor as well as the joint influence due to interactions. While local SA typically uses OAT sampling, global SA can use either OAT or AAT strategies. In general, AAT methods provide a better characterization of interactions between input factors. The drawback of AAT methods is that they typically require more extensive sampling and therefore a higher number of model evaluations (Pianosi et al. 2016).

In the next sections, a general classification of the methods that can be applied to mathematical programming and optimization is given. These can involve post-optimal SA for linear programming, and perturbation/statistical methods for scenario analysis.

#### Post-optimal Analysis of Linear Programming

From the point of view of linear programming (LP), the SA (also known as parametric analysis) is a method that allows searching the effects produced by the changes in the values of the different parameters on the optimal solution. It is necessary to remember that changes in the primal solution automatically have an impact in the dual model; then, it is possible to choose which model (primal or dual) will be used for analyzing the effects. SA for LP identifies the sensitive parameters by determining the range or admissible variation gap for the different coefficients of the problem in which the current optimal solution remains as feasible as optimal in order to estimate/treat the sensitive parameters with more precision. The SA for LP is developed as part of the post-optimization stage that studies how the optimality conditions of the current solution is affected when one modification or change is applied to a parameter (coefficient) in the problem. Moreover, it allows establishing the solution when new variables or constraints are introduced to the problem. This method could be used for mapping purposes and could be classified as qualitative, local, OAT one. Although SA theory is well developed in linear programming, efforts are still being made to handle the integer programming case, mainly because of the lack of optimality criteria for the integer optimization problems (Jia and Ierapetritou 2004). By the use of commercial software and algorithms, modifications in the main algorithm are not possible to be implemented. For this reason, the SA for LP for mixed integer problems is rarely used since other scenario analysis or statistical methodologies are widely applied.

#### OAT Perturbation Methods for Scenario Analysis

According to our knowledge regarding the SC problems at strategic level, the most used methodology for SA is the scenario analysis through perturbation methods (PM) (this can be also placed in the category of statistical methods). This is one of the simplest methods for local SA and is used for screening purposes. With PM, the model is analyzed in order to derive more meaningful business insights for managers in making resource planning decisions and to provide the stakeholders with a comprehensive framework of scenarios according to which targeting guidelines, regulation, and policy strategies can vary. PM varies the input factors of the optimization model from their nominal values OAT and assesses the impacts on the optimization results via visual inspection, for example, by pair-comparison of nominal and perturbed inputs (Pianosi et al. 2016). A way to perform this analysis is for example by changing the most important input parameters at several levels (e.g., nominal, low, or high). The optimizations are run in a pre-established order to know the impact on the optimal solution. This approach is qualitative and the results can be displayed in graphical ways (e.g., Tornado plots). One advantage of this tool is that it is easy to implement and no need of additional specialized software is required but it can be coupled with more sophisticated statistical tools. A major disadvantage of this analysis is that it fails to detect interactions between the factors (Karlsson and Söderström 2002). The number of experiments is another drawback.

#### Statistical Methods

The performance of SA through statistical methods can use several techniques. Some examples of these methods are as follows: correlation and regression analysis for screening (e.g., Morris OAT screening (Morris 1991)), Monte-Carlo filtering (for mapping), variance-based methods (quantitative methods; e.g., FAST and Sobol (Gan et al. 2014)). The majority of these methods are well adapted for computer experiments and simulation problems. Depending on the type of statistical SA, the method can be coupled with sampling methods to solve local or GSA. These are very sophisticated techniques that (to the best of our knowledge) have not been applied to strategic problems of supply chain. Still, in this work, we are not only interested in screening the main input factors of the HSC but also in investigating the interactions of the parameters. A statistical technique that could fit to our problem is the design of experiments (DOE). The DOE can be used for simulation and optimization problems (e.g., Shang et al. (2004), Dellino et al. (2010), Kleijnen (2005), Karlsson and Söderström (2002), Longo (2011), and Hussain et al. (2012)). It is useful for parameter screening and interaction analysis. An “experimental plan” is followed by the optimization of the objective function to measure the system performance. The most common initial and final optimization designs of experiment are called the screening design (through factorial design) and the response surface method (Uy and Telford 2009). According to (Kleijnen 2005), quantitative verification and validation may use DOE.

### Sensitivity Analysis for HSC

Once this general overview of all the available SA methods has been given, it is possible to identify the type of SA to be implemented for the HSC model. There are few works that have applied SA to such models, all of them have used the OAT perturbation method and analyzed and discussed pre-established scenarios resulting in qualitative analyses. Johnson et al. (2008) studied the geographical sensitivity (economies of scale). A set of five demand penetration scenarios and several pathways for the SA related to the transportation type (pipeline and tanker trucks) and capacity (size and capacity of tanker truck liquefiers) has been considered; the pipeline costs and liquefier capacity were found as the most sensitive parameter. Electricity price, discount rate, and average refueling station size were also analyzed parameters. The study reported in Liu et al. (2012) focuses on the analysis of $H_2$ demand from $H_2$ FCEV and the related cost of hydrogen in Ontario. Three potential $H_2$ demand scenarios over a long time period (2015–2050) have been investigated. SA was implemented to investigate the uncertainties of electricity price, water price, energy efficiency of electrolysis, and plant life.

From the analyzed parameters, the electricity price was identified as a high sensitive input. Another example is given by Yang and Ogden (2013) who studied a number of sensitivity scenarios to investigate the cost and emissions implication of altering policy constraints, technology and resource availability, and modeling decisions. A number of scenario inputs/constraints are varied (e.g., CCS available, coal allowed with or without CCS, biomass availability, demand trajectory, and carbon taxes) to understand how policy constraints and other input assumptions can influence the modeling results. Murthy Konda et al. (2011) concluded that the production cost is strongly correlated to the feedstock prices (with high fluctuations) which remain the biggest contributor. The geographical sensitivity has also being analyzed with its effect of territory breakdown and economy of scale in De-León Almaraz et al. (2015).

In this work, the valuable results obtained by the abovementioned studies are taken into account and will serve to target the set of parameters to be studied in our SA. From these studies, two types can be found, those related to the capital cost (e.g., facilities and transportation investments) and the others related to operational cost (e.g., electricity and feedstock prices, and operational efficiency); in all the cases, demand plays a major role; indeed, the mathematical model of the HSC is demand driven; this means that it is possible to conclude intuitively that this input parameter will have an important effect in the response, but its quantification as well as the interactions of this parameter with other sensitive ones have not been analyzed yet. In this paper, the OAT approach that has been applied to other HSC SA works has not been considered. In other fields of supply chain management, various works have efficiently used DOE methodology for parameter screening.

In this perspective, this work develops a sensitivity analysis by the use of DOE methodology to investigate the interaction and statistical significance of important parameters over the response variable (TDC). To the best of our knowledge, this is the first work that proposes such a methodology for the HSC model. With this analysis, the economic criterion can be deeply assessed and some modifications could take place. Some main questions that arise from the previous studies are as follows:

- Which of the cost types (capital or operational) is impacting more the HSC deployment for a long-term time horizon?
- What are the important factors that impact the TDC?
- Is the current cost optimization (by minimizing the TDC) representative enough considering the parameters uncertainty?
- What are the main parameter interactions for the HSC model?

The remainder of this paper is organized as follows: Section 2 is devoted to present the general model of the HSC to explain the TDC function and display all their terms. Section 3 introduces the DOE methodology and gives a brief description of important statistical tools related to this method (i.e., factorial design and response surface methods) and presents the optimization strategy. In Section 4, the case study of the former Midi-Pyrénées region treated in De-León Almaraz et al. (2014) (now included in the Occitanie region) is described, and from the literature review and our previous results, hypothetical important parameters are analyzed to create a set of factors proposed for the DOE study. Section 5 is devoted to the application of the methodology and the results are examined. The experiment databases are also presented for a two-level full factorial and response surface designs. Finally, conclusions and perspectives are proposed.

## Mathematical HSC Design Model

The HSC design approach has been extensively presented in De-León Almaraz et al. (2014) and is based on the works developed by Almansoori and Shah (2009, 2012), dedicated to the optimal TDC of the HSC through MILP (Fig. 2). The items of a HSC are shown in Fig. 1. In the proposed formulation, hydrogen can be produced from an energy source $e$, delivered in a specific physical form $i$, such as liquid or gaseous, produced in a factory type $p$ involving different production technologies, stored in a reservoir unit $s$ and distributed by a transportation mode $l$ from one district or grid $g$ to another $g'$ (with $g'g$). The facilities have different sizes $j$ (e.g., small, medium, and large). A multi-period optimization approach has been carried out with the objective of minimizing the criteria on the entire time horizon $t$. For the sake of brevity, only the key points of the approach are highlighted in what follows; the mathematical model is also developed in the supplementary material.

### Decision Variables

The design decisions are based on the number, type, capacity, and location of production and storage facilities as well as the number and the type of transport units required, and the flow rate of hydrogen between locations. The 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.

### Constraints

The involved constraints are related to demand satisfaction, the availability of energy sources, production facilities,

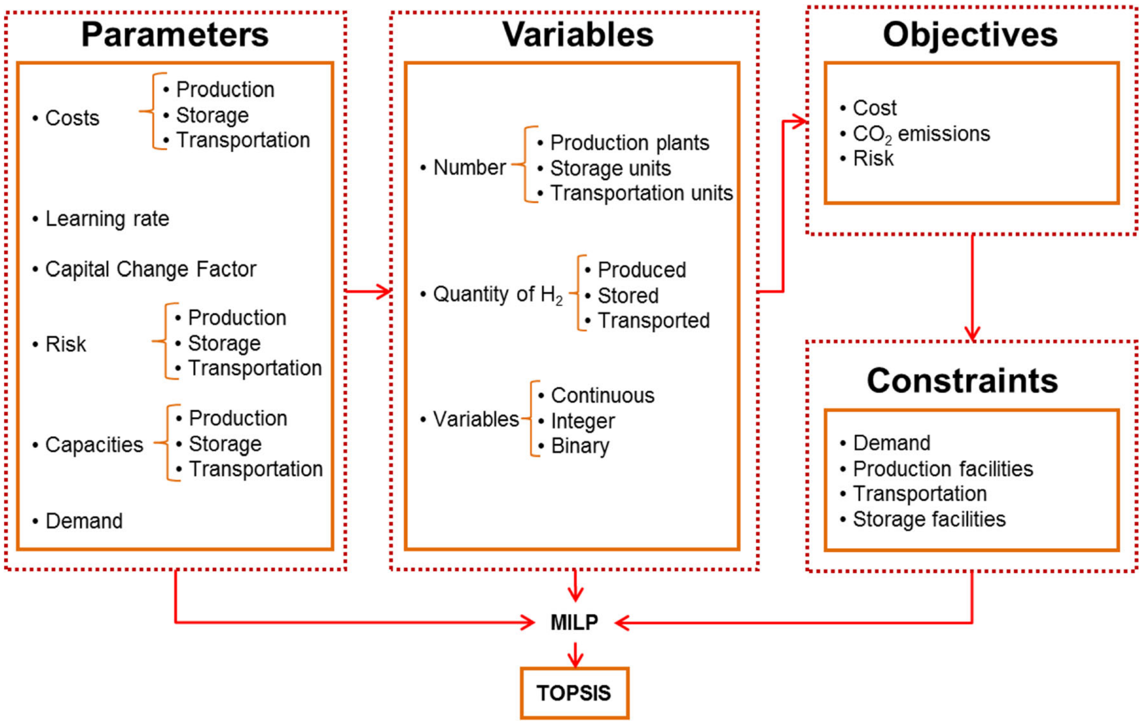


**Fig. 2** The HSC model proposed by De León Almaraz et al. (2014)

storage units, transportation modes and flow rates. Again, for reason of brevity, only a short description of the key constraints is given in this section (see De León Almaraz (2014) for more information).

### Demand

Each grid $g$ has its own deterministic demand. It must be fulfilled either by production facilities established within a particular grid (local production), or by importing products from other neighboring grids. Besides, the demand in the grid $g$ satisfied by neighboring grids is equal to the total flow imported to that grid by all types of transportation modes. Finally, the total grid demand ($DT_{ig}$) must equal the demand satisfied by the local production plus the demand imported from other grids.

### Energy Source Constraints

The average availability of primary energy sources $e$ in a grid $g$ during time period $t$ is given as a sum of the initial availability of energy sources, the imported energy sources, and the rate of consumption of these. One important parameter here is the rate of utilization of primary energy source $e$ by plant type $p$ and size $j$ which can be associated with the process efficiency and has a direct impact on the operational cost.

### Production and Storage Constraints

The total number of production facilities type $p$ and size $j$ installed in $g$ in the time period $t$ is determined by the sum of the initial number of plants ($NP_{pijgt}$) and the number of new units in the period $t$ ($IP_{pijgt}$). For all the other periods, the establishment of new production facilities takes into account the production plants installed in the previous time periods. In the case of new electrolysis plants that use renewable energy $e$, they can only be established where renewable energy $e$ is available. The installation of new storage units ($IS_{sigt}$) is constrained by the availability of current storage facilities of type $s$ and size $j$ storing product form $i$ in grid $g$ established in the previous time periods ($NS_{sigt}$).

### Transportation and Refueling Station Constraints

There must be a continuous flow of hydrogen between different grids in order to satisfy the required demand. The flow of hydrogen form $i$ from grid $g$ to a different grid $g'$ will only exist if the transportation mode is established. Thus, there is always a minimum and a maximum flow rate of hydrogen needed to justify the establishment of a transportation mode between two grids in the network. The flow of a product form $i$ between different grids can only occur in one direction. Besides, a particular grid can only import $H_2$ from neighboring grids or export $H_2$ to other grids (only one condition can be satisfied). The number of refueling stations within a grid *g* dispensing a product form *i* depends on the total equivalent demand and the installed capacity of the fueling stations. To calculate the transportation pathway, binary variables are considered in the original model.

### Objective Function

As previously explained, the economic objective function considered by De-León Almaraz et al. (2014) is the TDC. The TDC of the whole HSC (expressed in $ per day) is calculated by the addition of several capital and operational costs as follows:

#### Capital Cost of Facilities and Transportation ($ per Day)

The facility capital cost ($FCC_t$) is expressed in Eq. 1. This expression involves the number of new plants (variable $IP_{pijgt}$) and storage facilities (variable $IS_{sijgt}$) to be installed in period *t* (both are integer variables). The capital costs for a plant *p* ($PCC_{pij}$) or a storage facility *s* ($SCC_{sij}$) are also displayed as parameters that are multiplied by the decision variables. The parameter of learning rate ($LR_t$) is also involved in this equation.

$$FCC_t = \sum_{i,g} \frac{1}{LR_t} \left. \sum_{p,j} PCC_{pij} IP_{pjigt} + \sum_{s,j} SCC_{sij} IS_{sijgt} \forall t \right) \tag{1}$$

#### Operating Cost of Facility and Transportation ($ per Day)

The facility operating cost (*FOC*) is constituted by the addition of two terms; the former is the product of the unit production cost ($ per kg $H_2$) and of the average production rate given in kilograms per day and the latter is the product of the unit storage cost ($ per kg $H_2$ per day) and the average storage rate in kilograms $H_2$. The transportation operating cost (*TOC*) is based on the determination of four costs related to transport units: fuel, labor, maintenance, and general costs. All these are continuous variables.

The *FOC* is related to the cost required to operate the production plants and storage facilities efficiently. It is obtained by multiplying the unit cost of production ($UPC_{pi}$) and storage ($USC_{si}$) by the corresponding amount of production ($PR_{pig}$) and storage ($ST_{ig}$).

$$FOC = \sum_{i,g} \left. \sum_{p} UPC_{pi} PR_{pigt} + \sum_{s,j} USC_{si} ST_{ig} \right) \tag{2}$$

#### Total Daily Cost ($ per Day)

The *TDC* is expressed in Eq. 3. In this expression, $FCC_t$ and $TCC_t$ (continuous variables) refer to facility and transportation capital cost (Section 2.3.1), respectively, in the time period *t*. $\alpha_{days}$ is a parameter related to the network operating period and *CCF* is the capital charge factor parameter as initially called in Almansoori and Shah (2006) (in years) and actually referring to the depreciation period. $FOC_t$ and $TOC_t$ are the facility and transportation operating cost variables (Section 2.3.2). Finally, $ESC_t$ refers to the cost of transportation of the energy source.

$$TDC = \sum_{t} \frac{FCC_t + TCC_t}{\alpha_{days} CCF} + FOC_t + TOC_t + ESC_t \tag{3}$$

## Methods and Tools

### Design of Experiments

The Design of Experiments was proposed in Fischer (1937). This method is based on the right planning, design, and execution of tests to conduct experiments efficiently. The DOE is widely used in product and process development, enhancement, and optimization; it is also largely used for screening, optimization, and robustness testing. In the case of this research, the SA can be developed by the screening of important factors through the DOE methodology because it is efficient compared to the OAT approach. Indeed, screening design allows changing factor levels simultaneously and also to find the interactions among the factors with few experiments. Three main components are involved in the DOE process, i.e., the factors, levels, and response. The factors are the sources that have some impact in the results or response. The levels are the values of each factor. The response corresponds to the results of the system. The methodology starts with the specification of the input conditions: the number of factors and their ranges, the number of responses, and the experimental objective. The experimental design can then be created and performed. Once collected, these data are investigated using regression analysis. This gives a model relating the changes in factors to the changes in responses. The model will indicate which factors are important and how they combine in influencing the responses. Typically, DOE encompasses three experimental objectives (Eriksson 2008):

1. *Screening design*: by using factorial designs which studies the response of every combination of factors and factor levels. Full factorial designs give the basis for all the classical experimental designs used in screening but also for optimization, and robustness testing. One of the most

common is the $2^k$ factorial design, where two levels are taken for each factor, respectively, low and high. These two levels are represented by the numbers of − 1 and + 1.

2. *Optimization*: to extract in-depth information about the few dominating factors. A quadratic model is flexible and may closely approximate the "true" relation between the factors and the responses. The response is modeled and can be displayed through a response surface plot. This approach is also known response surface modeling (RSM). For some factors and responses, a positive (respectively negative) correlation may exist. These relationships are conveniently investigated by fitting a quadratic regression model. This part is very important for our study because it allows identifying the factor levels that satisfy certain requirements on the model and the relationship between different factors (Meyer and Krueger 1997).
3. *Robustness testing*, which is useful in process and product design as a final test to ensure quality.

The solution set consists of an ANOVA (ANalysis Of VAriance) table, the ANOVA analysis is a tool used to test the differences between two or more factors (Mathews 2005). The essential purpose of performing an ANOVA method is to analyze if any statistical significant difference exists between the different factors or variables.

### Factorial Design Method

A factorial design method offers a tool making it possible to detect interaction effects (Box et al. 1978) in (Karlsson and Söderström 2002). The factorial design method tends to increase in size when many factors are to be evaluated but it is possible to reduce this problem by using a fractional factorial design method. The number of experiments, using a plain factorial design method, depends on the number of factors and the number of levels to be studied, according to $p^k$, where $p$ is the number of levels and $k$ is the number of factors to be studied. From this, it is possible to calculate $k$ main effects and two-factor interactions (even more). The selection of an appropriate regression model is part of the problem formulation. Three main types of polynomial models are distinguished: linear, interaction, and quadratic models. In screening, either linear or interaction models are used (Eriksson 2008).

### Response Surface Methodology

RSM was introduced by Box and Wilson (1951). RSM is often used to refine models after the important factors have being identified using factorial designs. In RSM, it is important to get good regression models. There are several classical RSM design families: i.e., central composite, Box-Behnken, and three-level full factorial designs (Eriksson 2008). Box-Behnken designs usually have fewer design points than central composite designs; thus, they are less expensive to run with the same number of factors. They can efficiently estimate the first- and second-order coefficients; however, they cannot include runs from a factorial experiment (Minitab 17 2016). Central composite designs (CCD) can fit a full quadratic model. They are often used when the design plan calls for sequential experimentation because these designs can include information from a correctly planned factorial experiment. A central composite design is the most commonly used response surface designed experiment and is especially useful in sequential experiments because it is possible to build on previous factorial experiments by adding axial and center points (Minitab 17 2016).

### TDC Optimization Stage and SA

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) ≤ 0. The mono-objective optimization is applied by the minimization of the TDC. The global MILP model can be formulated in a concise manner as follows:

$$\begin{array}{l} \mathrm{Minimize}\{\mathrm{TDC}\} \\ \mathit{Subject\ to}: \\ \mathrm{h(x,y)} = 0 \\ \mathrm{g(x,y)} \leq 0 \end{array} \left\{ \begin{array}{c} \mathit{Demand\ satisfaction} \\ \mathit{Capacity\ limitations} \\ \mathit{Distribution\ network\ design} \\ \mathit{Site\ allocation} \\ \mathit{Non\text{-}negativity\ constraints} \end{array} \right\}$$
$$x \in R^n, y \in Y = \{0,1\}^m, z \in Z^+$$

The problem is treated with GAMS 23.9 (Brooke et al. 1992) and solved by CPLEX 12. According to the experimental plan proposed through the DOE methodology, the changes of some parameters will be performed in the HSC model code and the optimizations will be run until the whole set of experiments is complete.

## Case Study

### General Description

The case study refers to the implementation of a HSC in the Midi-Pyrénées region, in France (De-León Almaraz et al. 2014). A deterministic demand of hydrogen is considered, including fleets such as buses, private and light-good-vehicles and forklifts at 2010 levels. Market demand scenarios selected for this project were based on McKinsey&Company (2010) and Bento (2010). From these studies and the involved assumptions, two scenarios with two levels of demand (low and optimistic) for FCEV penetration were developed but only the low demand scenario was evaluated in De León Almaraz (2014). The problem is defined as multi-period and the time horizon considered is 2020–2050 with a time step of 10 years.

## Choice of Factors, Levels, and Response

In this work, a local sensitivity is performed through DOE where the response variable is the *TDC* (Eq. 3). Let us remember that for a complex system model with a lot of parameters, qualitative SA methods can be first used for a rough parameter screening (pre-screening), which will prune the most insensitive parameters with low evaluation costs. Then, quantitative SA methods can be adopted for a further SA of this simplified system model (Gan et al. 2014). We have decided to make a pre-screening of key parameters based on the conclusion of the previously developed SA for the HSC in the dedicated literature (see Section 1.2 and the remaining of this section). Some of these key parameters will be studied to verify if they are really sensitive and at what level and also to find major interactions between them. The list of potential factors is given below.

### Demand

A sensitivity analysis of the demand parameter is carried out in various HSC SAs (e.g., Ren and Gao (2010), Yang and Ogden (2013), Murthy Konda et al. (2011), Johnson et al. (2008)). The demand in the HSC models has been studied only in scenario-based analysis (Ball and Wietschel 2009). Demand scenarios are used to study the market for demand and supply site activities. The introduction of $H_2$ in highly populated areas leads to economies of scale of $H_2$ production (Ball et al. 2007). The geographical scale (economies of scale) and demand penetration scenarios result tends to a change in the centralization degree and have a high impact in the cost of the HSC (De-León Almaraz et al. 2015).

### Capital and Operational Costs

A common approach to measure the SA is the comparison of capital (CapEx) and operational cost (OpEx). This has been analyzed for different types of supply chains or facilities technologies. (Swanson et al. 2010) compare capital and production costs of two biomass-to-liquid production plants. Three scenarios that represent the range of estimates for cost growth and plant performance were considered: most probable, optimistic, and pessimistic. For this work, the most influential parameter is total CapEx because it affects the capital depreciation, average income tax, and average return on investment. Kaldellis et al. (2005) conducted a study to find the key factors of a SC; they found that the installation capacity factor, the local market electricity price annual escalation rate, and the reduced first installation cost are found to be the parameters that mostly affect the viability of similar ventures. The key parameters are the investment costs for production plants, storage and transportation units, the learning rate, and the payback period.

### Feedstock

For operational cost, the feedstock, the production efficiency, and the electricity costs have been reported as key parameters. According to Ball et al. (2007), the infrastructure buildup for the HSC is strongly influenced by the assumed feedstock prices. The economic performance of all the SCs is very sensitive to the prices of raw materials and products, which usually change with time (Vlysidis et al. 2011). According to the technology, the feedstock price can be considered as the cost of raw materials or in the case of electrolysis as water and electricity prices. Zhang et al. (2003) concluded that the prices of feedstock and plant capacity are the most significant factors affecting the economic viability of biodiesel SC. In the specific case of the HSC, in the SA performed by Murthy Konda et al. (2011), the feedstock remains the biggest contributor with 40% share of the cost split. Yang and Ogden (2013) varied the biomass availability. Electricity price for electrolysis production has been studied in Johnson et al. (2008). In Liu et al. (2012), the electricity price was concluded to be a high sensitive input. Mueller-Langer et al. (2007) show that the higher the share of electricity costs on total hydrogen production costs, the lower the influence of annual full load operation hours to these total costs. This parameter is not currently independently calculated in our model according to the energy source. The operational cost for electricity is the same for all the type of energy sources. In order to verify the sensitivity of this parameter, a modification in Eq. (2) is necessary to compute different electricity costs regarding the sources.

### Key Factors and Experiment Plan

Based on the abovementioned options, the pre-screened parameters for the HSC model proposed in this research are six and are listed below:

- Demand (*DT*)
- Capital change factor (*CCF*)
- Storage capital cost (*SCC*)
- Production capital cost (*PCC*)
- Learning rate (*LR*)
- Unit production cost (*UPC*)

The *CCF*, *SCC*, *PCC*, and *LR* are all related to investment cost. Besides, the operational cost analysis could be affected by *UPC* and the *LR*. In both groups, the demand is likely to play an important role. The set of parameters has thus been studied (see Table 1) and a linear experiment is considered based on the investigation on a given combination of factors

**Table 1** Values of the factors in all the experiments

| Experiment (comments) | Type | Factors | Values | | | | |
|---|---|---|---|---|---|---|---|
| | | | | 1 | | + 1 | |
| 1. Fractional factorial design | $2^6$ | Demand (level)♦ | | a | | + b | |
| | | CCF (years) | | 3 | | 12 | |
| | | LR (%) | | 5 | | 18 | |
| | | PCC (%)♣ | | 25 | | 25 | |
| | | SCC (%)♥ | | 25 | | 25 | |
| | | UPC (%)♠ | | 25 | | 25 | |
| | | | $\alpha_{CCD}$ | 1 | 0 | + 1 | $+\alpha_{CCD}$ |
| 2. Response surface (central composite design) | $2^6$ square model | Demand (level)*♦ | $\alpha_1$ | *a* | 0 | + b | $\alpha_1$ |
| All the runs are the same as in experiment 1. Runs from 33 to 54 includes the central and axial points in order to develop a quadratic model | | CCF (years) | $\alpha_2 = 1$ | 3 | 7.5 | 12 | $\alpha_2 = 14$ |
| | | LR (%) | $\alpha_3 = 0$ | 5 | 11.5 | 18 | $\alpha_3 = 23$ |
| | | PCC (%)♣ | $\alpha_4 =$ 59.2 | 25 | 0 | 25 | $\alpha_4 = 59.2$ |
| | | SCC (%)♥ | $\alpha_4 =$ 59.2 | 25 | 0 | 25 | $\alpha_4 = 59.2$ |
| | | UPC (%)♠ | $\alpha_4 =$ 59.2 | 25 | 0 | 25 | $\alpha_4 = 59.2$ |

♦ Demand nominal values (kg $H_2$ per day per grid) available in Supplementary Material, Table 1. ♣ PCC nominal values ($) available in Supplementary Material, Table 2. ♥ SCC nominal values ($) available in Supplementary Material, Table 3. ♠ UPC nominal values ($ per kg $H_2$) available in Supplementary Material, Table 4. $\alpha_1 = 1.80$, $\alpha_2 = 1.44$, $\alpha_3 = 1.77$, $\alpha_4 = 2.36$

with lower and upper bounds for each factor. The response TDC will be measured in $ per kilogram $H_2$ per day and the null and alternative hypotheses are defined as follows:

$$H_0: \ \mu_{TDC1} = \mu_{TDC2} = \ldots = \mu_{TDCk}$$
$$H_A: \ \mu_{TDC1} \neq \mu_{TDCi'}$$
$$\mu_{TDCi'} = \mu_{TDC} + \delta_i$$

where

$\mu_{TDC}$ average TDC before any treatment, with $n = 1$
$\delta_i$ estimated effect to $\mu_{TDC}$ in treatment $i$

To compare the media and variability between experiments, the $F$ statistic is calculated and presented in the ANOVA table. If the $p$ value is small enough ($p$ value < $\alpha = 0.05$), $H_0$ is rejected concluding that the data provide evidence of a difference in the population mean at least for a pair of factors. It is important to highlight that the classic DOE requires a given number of observations ($n$: number of samples) and a random assignation of experiments with replications to measure the variability due to external factors but, for our case, $n$ is assumed to be 1 because we are using an exact optimization tool (CPLEX algorithm) for deterministic data, i.e., the different levels for a factor are modified in the model database before each optimization run and the result is an optimal value. Thus, the order of the optimization runs does not have any impact in the other DOE calculations and replications are not needed.

In a second stage, the response surface through CCD methodology is applied for the same problem. In this stage, it is necessary to identify the axial points ($\alpha_{CCD}$), for the response surface to provide the orthogonal blocking and whenever possible rotatability. Due to the problem size, a fractional CCD (half design) with 8 cube points and 2 axial points is proposed. (Minitab Inc. 2000) suggests $\alpha_{CCD} = \pm\ 2.366$ (where $\alpha_{CCD}$ is the distance of each axial point). In our case study, some values related to demand, LR, and CCF are negative for the axial point $-2.366$; in real problems, these values are not reasonable; thus, a specific calculation for $\pm\alpha_{CCD}$ for those three parameters is estimated independently affecting lightly the rotatability but allowing to observe the general behavior of the model in a good enough level to draw general conclusions (see Table 1). The values for each factor are listed in the next sections.

**Demand** The demand (expressed in kg of $H_2$ per day) is required in 22 different districts during 4 time periods (2020, 2030, 2040, and 2050). One base scenario is proposed (level zero). Demand values are called (− *a*) and (+ *b*) for the lower and upper levels, respectively. A margin of ± 50% is taken into account for the factorial design. Every grid has its own deterministic demand. The values used in the experiments are the ones presented in De-León Almaraz et al. (2014). For the demand parameter, an $\alpha_{CCD} = \pm 1.8$ is assumed to avoid negative or zero values for the lower bound remaining with a minimum bound equivalent to 10% of the level zero of demand; this means to retain a very low demand level but still positive to keep an optimization problem (levels are presented in Table 1, and nominal values in Supplementary Material Table 1).

**Table 2** Experiment 1. Treatment matrix for the factorial design and results for the response TDC

| Test | Demand | CCF | LR | PCC | SCC | UPC | Response (TDC, \$ per day) $1 \times 10^6$ |
|---|---|---|---|---|---|---|---|
| 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1.54 |
| 2 | 1 | 1 | 1 | 1 | 1 | 1 | 2.71 |
| 3 | 1 | 1 | 1 | 1 | 1 | 1 | 0.75 |
| 4 | 1 | 1 | 1 | 1 | 1 | 1 | 2.17 |
| 5 | 1 | 1 | 1 | 1 | 1 | 1 | 1.70 |
| 6 | 1 | 1 | 1 | 1 | 1 | 1 | 2.88 |
| 7 | 1 | 1 | 1 | 1 | 1 | 1 | 0.80 |
| 8 | 1 | 1 | 1 | 1 | 1 | 1 | 2.23 |
| 9 | 1 | 1 | 1 | 1 | 1 | 1 | 1.62 |
| 10 | 1 | 1 | 1 | 1 | 1 | 1 | 2.93 |
| 11 | 1 | 1 | 1 | 1 | 1 | 1 | 0.77 |
| 12 | 1 | 1 | 1 | 1 | 1 | 1 | 2.23 |
| 13 | 1 | 1 | 1 | 1 | 1 | 1 | 1.99 |
| 14 | 1 | 1 | 1 | 1 | 1 | 1 | 3.50 |
| 15 | 1 | 1 | 1 | 1 | 1 | 1 | 0.88 |
| 16 | 1 | 1 | 1 | 1 | 1 | 1 | 2.38 |
| 17 | 1 | 1 | 1 | 1 | 1 | 1 | 1.22 |
| 18 | 1 | 1 | 1 | 1 | 1 | 1 | 2.98 |
| 19 | 1 | 1 | 1 | 1 | 1 | 1 | 0.90 |
| 20 | 1 | 1 | 1 | 1 | 1 | 1 | 1.73 |
| 21 | 1 | 1 | 1 | 1 | 1 | 1 | 1.52 |
| 22 | 1 | 1 | 1 | 1 | 1 | 1 | 3.50 |
| 23 | 1 | 1 | 1 | 1 | 1 | 1 | 1.02 |
| 24 | 1 | 1 | 1 | 1 | 1 | 1 | 1.86 |
| 25 | 1 | 1 | 1 | 1 | 1 | 1 | 1.49 |
| 26 | 1 | 1 | 1 | 1 | 1 | 1 | 3.55 |
| 27 | 1 | 1 | 1 | 1 | 1 | 1 | 0.98 |
| 28 | 1 | 1 | 1 | 1 | 1 | 1 | 1.87 |
| 29 | 1 | 1 | 1 | 1 | 1 | 1 | 1.60 |
| 30 | 1 | 1 | 1 | 1 | 1 | 1 | 3.69 |
| 31 | 1 | 1 | 1 | 1 | 1 | 1 | 1.03 |
| 32 | 1 | 1 | 1 | 1 | 1 | 1 | 1.91 |

**Capital Change Factor** A *CCF* value of 12 years (high level) is used for the Midi-Pyrénées territory under the assumption that a new infrastructure system is to be installed without subsides with low demand De-León Almaraz et al. (2014). In our view, the level is of 3 years used in Almansoori and Shah (2006) is not realistic for the high level of investment required. For lower and higher axial points, *CCF* nominal values are 1 and 14 years, respectively, equivalent to a value of $\alpha_{\mathrm{CCD}} = \pm 1.44$ (see Table 1).

**Learning Rate** The LR is a cost reduction for technology and manufacturers that results from the accumulation of

**Table 3** ANOVA table of experiment 1

| Source | DF | Seq SS | Adj SS | Adj MS | *F* | *P* value |
|---|---|---|---|---|---|---|
| Main effects | 5 | $2.31135 \times 10^{13}$ | $2.31135 \times 10^{13}$ | $3.85226 \times 10^{12}$ | 7673.35 | 0.000 |
| 2 way interactions | 15 | $7.93169 \times 10^{11}$ | $7.93169 \times 10^{11}$ | $5.28779 \times 10^{10}$ | 105.33 | 0.009 |
| 3 way interactions | 8 | $9.07251 \times 10^{11}$ | $9.07251 \times 10^{11}$ | $1.1340 \times 10^{11}$ | 225.90 | 0.004 |
| Residual error | 2 | $1.00406 \times 10^{9}$ | $1.00406 \times 10^{9}$ | $5.02030 \times 10^{8}$ | | |
| Total | 31 | $2.48150 \times 10^{13}$ | | | | |

experience during a time period. From (van der Zwaan 2009), LR values for electrolysis and SMR vary from 5 to 18% for a period of 10 years. These values are used for the two basic levels of this factor. For lower and higher axial points, *LR* nominal values are 0 and 23%, respectively, equivalent to a value of $\alpha_{\mathrm{CCD}} = \pm 1.77$ (presented in Table 1, and Supplementary Material Table 2).

**Production/Storage Capital Costs and Unit Production Cost** These three parameters have been grouped in this section because they share the same low and high percentage values as well as the lower and upper bounds for axial points (see Table 1). The PCC is the capital cost of a plant to produce hydrogen ($ US). Three types of production plants (i.e., SMR), and two types of electrolysis plants (centralized or distributed units) with three sizes (small, medium, and large) are considered. From the values proposed by (Almansoori and Shah 2009), a margin of ± 25% is used to estimate high and low levels for the experiments while $\alpha_{\mathrm{CCD}} = \pm 2.366$ represents a ± 59.2% cost increase/decrease regarding the zero level for axial points (Supplementary Material Table 3). The SCC is the capital cost of a storage tank (expressed in $ US). Four types of storage facilities are considered (i.e., mini, small, medium, and large for the Midi-Pyrénées case). Similar to the PCC case, ± 25% margin is taken into account for high/low levels and same values for $\alpha_{\mathrm{CCD}}$ are considered (nominal values in Supplementary Material Table 4). Finally, the UPC ($ per kg $H_2$) is the unit production cost

**Table 4** Coefficients and *P* values of the experiments

a) Experiment 1

| Term | Coef ($1 \times 10^3$) | *P* |
|---|---|---|
| Constant | 1935.728 | 0.000 |
| Demand | 697.979 | 0.000 |
| CCF | 466.331 | 0.000 |
| LR | 96.033 | 0.002 |
| PCC | 91.155 | 0.002 |
| SCC | 6.548 | 0.240 |
| UPC | 9.156 | 0.147 |
| Demand×CCF | 119.105 | 0.001 |
| Demand×LR | 15.983 | 0.056 |
| Demand×PCC | 34.189 | 0.013 |
| Demand×SCC | 11.522 | 0.101 |
| Demand×UPC | 27.621 | 0.020 |
| CCF×LR | 50.527 | 0.006 |
| CCF×PCC | 54.522 | 0.005 |
| CCF×SCC | 50.089 | 0.006 |
| CCF×UPC | 12.912 | 0.083 |
| LR×PCC | 0.646 | 0.885 |
| LR×SCC | 7.118 | 0.214 |
| LR×UPC | 1.279 | 0.777 |
| PCC×SCC | 4.532 | 0.371 |
| PCC×UPC | 2.432 | 0.602 |
| SCC×UPC | 0.233 | 0.958 |
| Demand×CCF×LR | 13.386 | 0.078 |
| Demand×CCF×PCC | 20.474 | 0.035 |
| Demand×CCF×SCC | 159.735 | 0.001 |
| Demand×CCF×UPC | 47.226 | 0.007 |
| Demand×LR×PCC | 0.050 | 0.991 |
| Demand×LR×SCC | 0.203 | 0.964 |
| Demand×LR×UPC | 2.298 | 0.620 |
| Demand×PCC×SCC | 1.472 | 0.746 |
| $R^2 = 100.00\%$ | | |

b) Experiment 2

| Term | Coef ($1 \times 10^3$) | *P* |
|---|---|---|
| Constant | 2115.784 | 0.000 |
| Demand | 681.632 | 0.000 |
| CCF | 537.902 | 0.000 |
| LR | 40.616 | 0.356 |
| PCC | 90.325 | 0.047 |
| SCC | 82.782 | 0.067 |
| UPC | 66.833 | 0.134 |
| Demand×Demand | 81.033 | 0.037 |
| CCF×CCF | 219.017 | 0.000 |
| LR×LR | 47.051 | 0.213 |
| PCC×PCC | 51.073 | 0.177 |
| SCC×SCC | 48.420 | 0.200 |
| UPC×UPC | 62.434 | 0.102 |
| Demand×CCF | 119.105 | 0.026 |
| Demand×LR | 12.912 | 0.799 |
| Demand×PCC | 15.983 | 0.752 |
| Demand×SCC | 34.189 | 0.502 |
| Demand×UPC | 50.089 | 0.327 |
| CCF×LR | 27.621 | 0.587 |
| CCF×PCC | 50.527 | 0.323 |
| CCF×SCC | 54.522 | 0.287 |
| CCF×UPC | 11.522 | 0.820 |
| LR×PCC | 4.532 | 0.929 |
| LR×SCC | 7.118 | 0.888 |
| LR×UPC | 0.233 | 0.996 |
| PCC×SCC | 0.646 | 0.990 |
| PCC×UPC | 2.432 | 0.962 |
| SCC×UPC | 1.279 | 0.980 |
| $R^2 = 95\ 3\%$ | | |

originally taken into account in De-León Almaraz et al. (2014) based on Almansoori and Shah (2009). Hydrogen can be produced using natural gas in SMR plants or using water and electricity in electrolysis facilities that are of two types, either centralized plants or distributed electrolysers installed in the refueling stations. Several types of energy sources can be considered in the model and differentiated by technologies, costs, and emissions. Yet, for simplicity purpose, the impact of the cost of the energy source was not considered. The design of experiments in this work proposes a UPC variation between ± 25% for its two basic levels and $\alpha_{CCD} = \pm 2.366$, i.e., ± 59.2% cost variation. (See Table 1 and Supplementary Material Table 5).

## Results and Discussion

The DOE was developed with MINITAB software version 14 (Minitab Inc. 2000). MINITAB is statistic software that helps to solve different kinds of statistical problems. The factors and the levels depend of the type of case that is analyzed. For example, for experiment 1, only the low and high levels were taken into account for a $2^6$ fractional factorial analysis. In experiment 2, the same experiment was treated using a response surface with central composite design.

### Experiment 1

The treatment matrix for the factorial design is presented in Table 2. For experiment 1, the fractional factorial design with a total of 32 treatments was studied. It must be emphasized that a reduced or fractional model (Burrill 1997) was used to reduce the computing effort and number of runs. As explained in Section 4.2.4, no replication is needed for our optimization problem since a gap in GAMS can be set and same results can be found in different machines. Results for the TDC response are also listed in Table 2. The statistical results are presented in the ANOVA table in Table 3. The influences of the six main factors and their interactions are evaluated. The data in the ANOVA table provide convincing evidence that the TDC is different for at least one pair of factors. From the results displayed in Table 4, it is possible to conclude that the demand, the CCF, the LR, and the PCC are the factors that are statistically significant; meaning that the $P$ value is lower than $\alpha = 0.05$ for a 95% confidence level. The significance of these parameters is also supported by the Pareto chart displayed in Fig. 3. It can be observed that the standardized effects are the $t$ statistics shown in the Session window of Minitab. The $t$ statistics are calculated by dividing each coefficient by its standard error (Coef/SE Coef). The reference line is calculated using lenth's pseudo-standard error (PSE). The pseudo-standard error is based on the concept of sparse effects, which assumes the variation in the smallest effects is because of

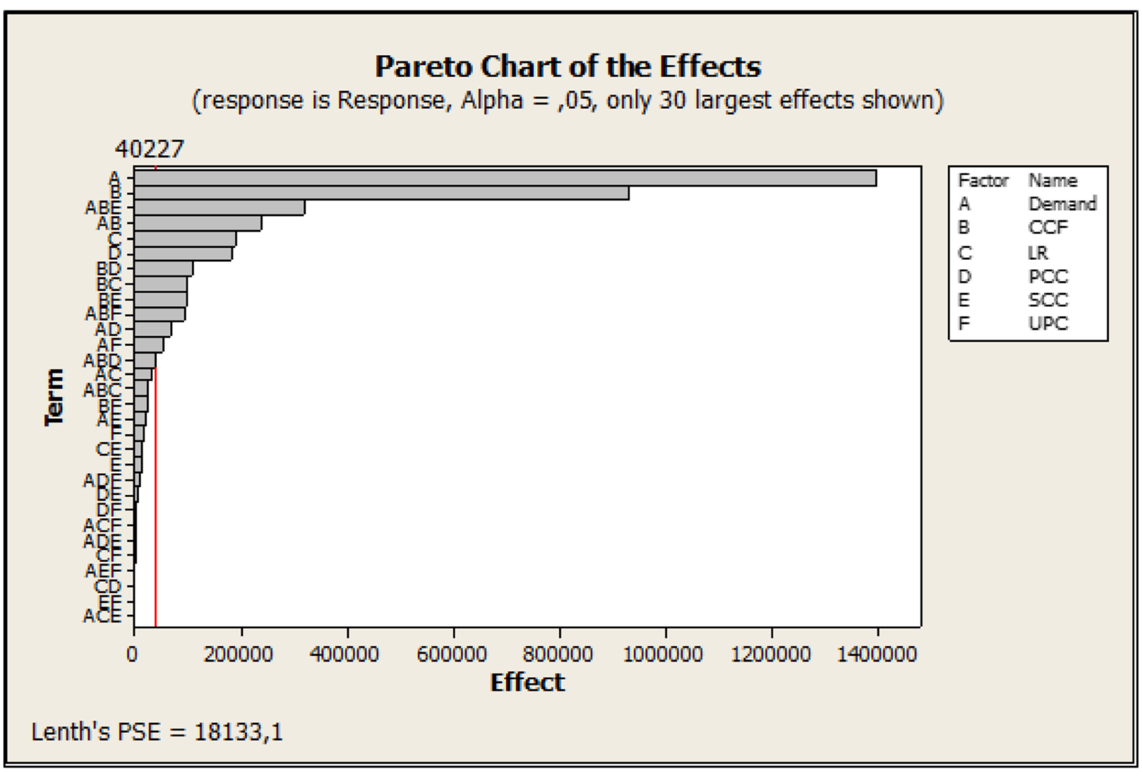


Fig. 3 Pareto chart of the factors in experiment 1

**Table 5** Experiment 2. Experimental design for the central composite design and response values

| Test | Demand | CCF | LR | PCC | SCC | UPC | Response (TDC, $ per day) $1 \times 10^6$ |
|---|---|---|---|---|---|---|---|
| 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1.54 |
| 2 | 1 | 1 | 1 | 1 | 1 | 1 | 2.71 |
| 3 | 1 | 1 | 1 | 1 | 1 | 1 | 0.75 |
| 4 | 1 | 1 | 1 | 1 | 1 | 1 | 2.17 |
| 5 | 1 | 1 | 1 | 1 | 1 | 1 | 1.70 |
| 6 | 1 | 1 | 1 | 1 | 1 | 1 | 2.88 |
| 7 | 1 | 1 | 1 | 1 | 1 | 1 | 0.80 |
| 8 | 1 | 1 | 1 | 1 | 1 | 1 | 2.23 |
| 9 | 1 | 1 | 1 | 1 | 1 | 1 | 1.62 |
| 10 | 1 | 1 | 1 | 1 | 1 | 1 | 2.93 |
| 11 | 1 | 1 | 1 | 1 | 1 | 1 | 0.77 |
| 12 | 1 | 1 | 1 | 1 | 1 | 1 | 2.23 |
| 13 | 1 | 1 | 1 | 1 | 1 | 1 | 1.99 |
| 14 | 1 | 1 | 1 | 1 | 1 | 1 | 3.50 |
| 15 | 1 | 1 | 1 | 1 | 1 | 1 | 0.88 |
| 16 | 1 | 1 | 1 | 1 | 1 | 1 | 2.38 |
| 17 | 0 | 0 | 0 | 0 | 0 | 0 | 2.07 |
| 18 | 0 | 0 | 0 | 0 | 0 | 0 | 2.07 |
| 19 | 0 | 0 | 0 | 0 | 0 | 0 | 2.07 |
| 20 | 0 | 0 | 0 | 0 | 0 | 0 | 2.07 |
| 21 | 1 | 1 | 1 | 1 | 1 | 1 | 1.22 |
| 22 | 1 | 1 | 1 | 1 | 1 | 1 | 2.98 |
| 23 | 1 | 1 | 1 | 1 | 1 | 1 | 0.90 |
| 24 | 1 | 1 | 1 | 1 | 1 | 1 | 1.73 |
| 25 | 1 | 1 | 1 | 1 | 1 | 1 | 1.52 |
| 26 | 1 | 1 | 1 | 1 | 1 | 1 | 3.50 |
| 27 | 1 | 1 | 1 | 1 | 1 | 1 | 1.02 |
| 28 | 1 | 1 | 1 | 1 | 1 | 1 | 1.86 |
| 29 | 1 | 1 | 1 | 1 | 1 | 1 | 1.49 |
| 30 | 1 | 1 | 1 | 1 | 1 | 1 | 3.55 |
| 31 | 1 | 1 | 1 | 1 | 1 | 1 | 0.98 |
| 32 | 1 | 1 | 1 | 1 | 1 | 1 | 1.87 |
| 33 | 1 | 1 | 1 | 1 | 1 | 1 | 1.60 |
| 34 | 1 | 1 | 1 | 1 | 1 | 1 | 3.69 |
| 35 | 1 | 1 | 1 | 1 | 1 | 1 | 1.03 |
| 36 | 1 | 1 | 1 | 1 | 1 | 1 | 1.91 |
| 37 | 0 | 0 | 0 | 0 | 0 | 0 | 2.07 |
| 38 | 0 | 0 | 0 | 0 | 0 | 0 | 2.07 |
| 39 | 0 | 0 | 0 | 0 | 0 | 0 | 2.07 |
| 40 | 0 | 0 | 0 | 0 | 0 | 0 | 2.07 |
| 41 | $\alpha$ | 0 | 0 | 0 | 0 | 0 | 0.39 |
| 42 | $\alpha$ | 0 | 0 | 0 | 0 | 0 | 3.39 |
| 43 | 0 | $\alpha$ | 0 | 0 | 0 | 0 | 5.33 |
| 44 | 0 | $\alpha$ | 0 | 0 | 0 | 0 | 1.81 |
| 45 | 0 | 0 | $\alpha$ | 0 | 0 | 0 | 2.13 |
| 46 | 0 | 0 | $\alpha$ | 0 | 0 | 0 | 2.03 |
| 47 | 0 | 0 | 0 | $\alpha$ | 0 | 0 | 1.88 |
| 48 | 0 | 0 | 0 | $\alpha$ | 0 | 0 | 2.23 |
| 49 | 0 | 0 | 0 | 0 | $\alpha$ | 0 | 1.94 |

**Table 5** (continued)

| Test | Demand | CCF | LR | PCC | SCC | UPC | Response (TDC, $ per day) $1 \times 10^6$ |
|---|---|---|---|---|---|---|---|
| 50 | 0 | 0 | 0 | 0 | $\alpha$ | 0 | 2.21 |
| 51 | 0 | 0 | 0 | 0 | 0 | $\alpha$ | 1.53 |
| 52 | 0 | 0 | 0 | 0 | 0 | $\alpha$ | 2.47 |
| 53 | 0 | 0 | 0 | 0 | 0 | 0 | 2.07 |
| 54 | 0 | 0 | 0 | 0 | 0 | 0 | 2.07 |

random error. Part of the main interactions in the model are as follows: demand × CCF × SCC, demand × CCF; CCF × PCC, CCF × LR, demand × CCF × UPC, and demand × UPC. The significant influence of the demand and CCF factors are therefore highlighted.

## Experiment 2

In experiment 2, the quadratic model of experiment 1 is developed by the evaluation of 5 levels using the central composite design. As previously explained in Section 4.2, the $\alpha_{\mathrm{CCD}}$ value is required for axial points. The experimental design and response values for experiment 2 are presented in Table 5. The statistical results are presented in the ANOVA table (Table 6). The influences of the six main factors and their interactions are evaluated. From the results displayed in Table 4, it is possible to conclude that the demand, the CCF, and the PCC are the factors that are statistically significant; however, some interactions in this quadratic model are also relevant: $Demand^2$, $Demand \times CCF$, and $CCF^2$. Although the lack-of-fit is significant, meaning that its $P_{\mathrm{value}}$ is smaller than the significance level of 0.05 (Table 6), this does not mean that the quadratic model is totally inadequate (Stat-Ease 2004). The resulted regression function is presented in Eq. (4). The $R^2$ of this experiment is 95.3% which means that a good representation of the model could be done by the use of the resulted regression function (Eq. 4). Moreover, this function allows to find the best levels for parameters when the response is optimized. The effects in the response for the $\pm\alpha_{\mathrm{CCD}}$ are shown in Fig. 4.

$$
\begin{aligned}
TDC = {} & 2115784 + 681632 Demand - 537902 CCF \\
& + 90325 PCC - 66833 UPC \pm 81033 (Demand)^2 \\
& + 219017 (CCF)^2 - 119105 (Demand)(CCF)
\end{aligned}
\quad (4)
$$

## Optimal Levels for each Factor

The results from the quadratic models are used to perform an impact analysis of the optimal levels of each factor. As previously highlighted, for experiment 1, the main factors are demand, CCF, LR, and PCC, five double interactions and one triple. But, if we take into account the quadratic model (experiment 2), only demand, CCF, and PCC are significant and the main interaction is between demand and CCF. The influence of UPC can also be visualized. From these observations, different experiments can be done for validation purpose. In this section, the base "original" case presented in De-León Almaraz et al. (2014) is compared with different factor level combinations for experiments 1 and 2 and finally the optimization response is performed in Minitab to find the best combination for a given target for TDC. The obtained results are displayed in Table 7 and the corresponding HSC configurations for 2050 are also given (Figs. 5, 6, 7, and 8). For experiment 1, an optimization in GAMS has considered the values

**Table 6** ANOVA table of experiment 2

| Source | DF | Seq SS | Adj SS | Adj MS | $F$ | $P$ value |
|---|---|---|---|---|---|---|
| Regression | 27 | $3.83724 \times 10^{13}$ | $4.01659 \times 10^{13}$ | $1.42120 \times 10^{12}$ | 17.31 | 0.000 |
| Linear | 6 | $3.34807 \times 10^{13}$ | $3.34807 \times 10^{13}$ | $5.58011 \times 10^{12}$ | 69.47 | 0.000 |
| Square | 6 | $4.09854 \times 10^{12}$ | $4.09854 \times 10^{12}$ | $6.83091 \times 10^{11}$ | 8.50 | 0.000 |
| Interaction | 15 | $7.93169 \times 10^{11}$ | $7.93169 \times 10^{11}$ | $5.28779 \times 10^{10}$ | 0.66 | 0.798 |
| Residual error | 24 | $1.92777 \times 10^{12}$ | $1.92777 \times 10^{12}$ | $8.03236 \times 10^{10}$ | | |
| Lack of fit | 17 | $1.92777 \times 10^{12}$ | $1.92777 \times 10^{12}$ | $1.13398 \times 10^{11}$ | $2.2265 \times 10^{7}$ | 0.000 |
| Pure error | 7 | 35,651 | 35,651 | 5093 | | |
| Total | 53 | $4.28338 \times 10^{13}$ | | | | |

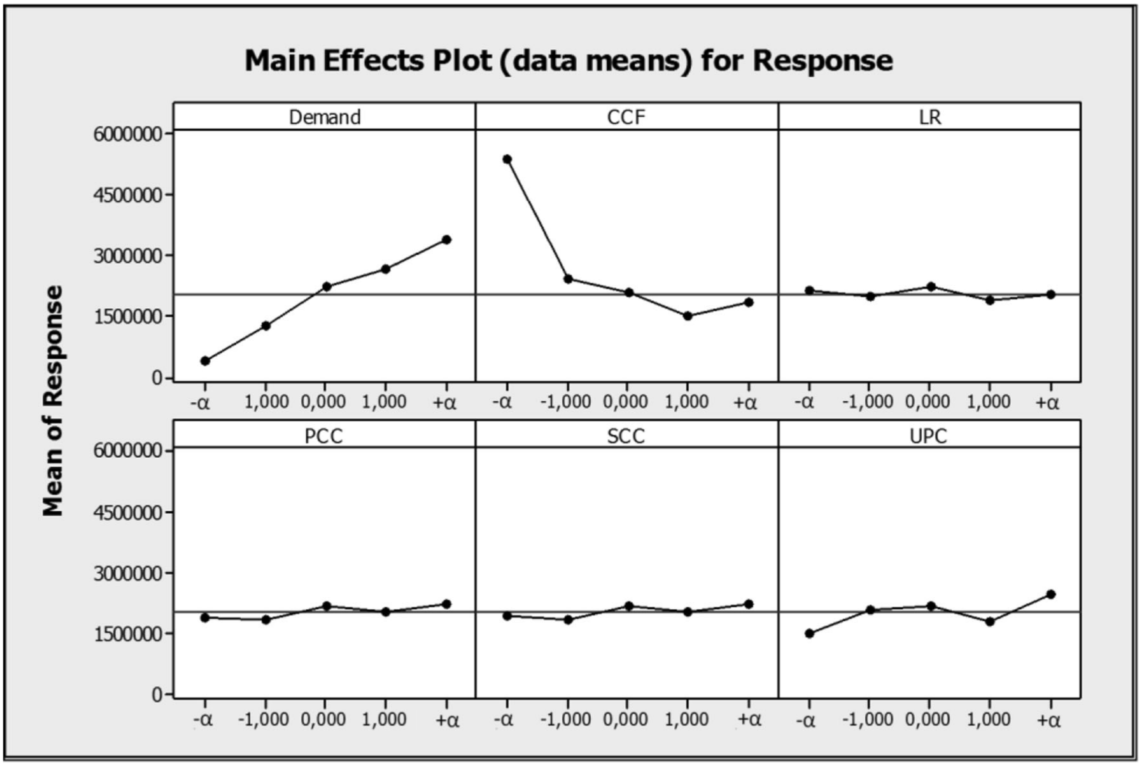


**Fig. 4** Main effect plots for the first quadratic model (Exp. 2)

of demand (− 1), CCF (+ 1), LR (+1), PCC (− 1), and UPC (− 1). For experiment 2, the following values for demand ($-\alpha_{CCD}$), CCF (+ 1), PCC (+ 1), and UPC ($-\alpha_{CCD}$) are considered. The results for "original," experiment 1, and experiment 2 are listed in Table 7. The optimization response is finally computed. Minitab proposes values of demand ($+\alpha_{CCD}$), CCF ($+\alpha_{CCD}$), LR ($-\alpha_{CCD}$), PCC ($-\alpha_{CCD}$), SCC ($\alpha_{CCD}$), and UPC ($-\alpha_{CCD}$) to achieve a TDC of $ 1890 million per day (equivalent to an average unit cost of $5.49 per kg $H_2$) (see Table 7).

Figure 5 represents the original distribution in 2050. It is clear that the distribution of the plants is not centralized. In experiment 1 (Fig. 6), it is observed that the cost in 2050 and the average cost are not close, which can be attributed to a low value of demand. Figure 7 shows the distribution of experiment 2. In 2050, the cost is higher than the value obtained in the original model and there is no transportation. Also, in the first period in this experiment, the cost per kilogram is too high (Table 7) due to the installation of all the plants and facilities in order to satisfy a very low demand. From the second period (2030), the cost decreases to the use of the already installed plant, thus reducing the capital cost. The mainly difference between experiments 1 and 2 is the impact of the demand. Even though in experiment 2 the TDC is low, the cost per kilogram is high. The opposite effect is observed with experiment 1. In order to obtain the optimization response, an average cost is fixed as an objective and is then converted into a TDC response value (Table 7). It must be said that the TDC and the average cost are not proportional. The result for 2050 of the optimization response is presented in Fig. 8. It can be highlighted that the average cost and the cost in all the periods are better that the values obtained in the original model, with a centralized distribution mainly with SMR production. This can be explained by the increase in both demand and CCF, and also by the UPC decrease.

## Discussion

In general, the demand is the most significant factor but CCF is also very significant in the current formulation of the HSC. If we take into account other factors, the PCC and LR are also relevant and UPC is significant for its interactions with each other. By taking into account the parameters and the uncertainty (e.g., the demand), the objective function of the HSC can be improved by considering other representative functions such as the net present value (NPV). In this section, the research questions addressed in Section 1.2 can be answered:

– *CapEx* vs. *OpEx*: for the case study that supports this methodological approach, considering that the geographical scale of Midi-Pyrénées is small compared to France, the capital cost has a larger impact in the first periods (2020 and 2030) than in the following ones, making the CCF a very important parameter. In the last periods (2040 and 2050), the operating cost drives the UPC. Yet, the UPC alone is not statistically significant but its interaction with

**Table 7** Cost optimization results of the HSC in the Midi-Pyrénées region and the best configurations

| | Original | | | | Experiment 1 | | | | Experiment 2 | | | | Optimization response | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Year | 2020 | 2030 | 2040 | 2050 | 2020 | 2030 | 2040 | 2050 | 2020 | 2030 | 2040 | 2050 | 2020 | 2030 | 2040 | 2050 |
| Demand (*t* per day) | 7.9 | 59.4 | 138.8 | 198.2 | 3.9 | 29.7 | 69.4 | 99.1 | 0.8 | 5.9 | 13.9 | 19.8 | 15.0 | 112.9 | 263.7 | 376.5 |
| Number of total production facilities | 25 | 43 | 43 | 43 | 22 | 45 | 46 | 46 | 22 | 22 | 29 | 36 | 33 | 34 | 35 | 35 |
| Number of total storage facilities | 22 | 41 | 71 | 116 | 26 | 37 | 70 | 97 | 24 | 46 | 58 | 80 | 51 | 73 | 80 | 99 |
| Number of transport units | – | 5 | 14 | 22 | 0 | 1 | 5 | 7 | 0 | 0 | 0 | 0 | 1 | 10 | 24 | 29 |
| Capital cost | | | | | | | | | | | | | | | | |
| Plants and storage facilities ($10^6$ \$) | 338.5 | 1081.5 | 171.2 | 127.8 | 194.2 | 554.7 | 146.9 | 55.0 | 173.8 | 76.1 | 77.1 | 51.8 | 717.5 | 1024.1 | 602.8 | 211.4 |
| Transportation modes ($10^6$ \$) | 0 | 2.5 | 7.0 | 11.0 | 0.0 | 0.5 | 2.5 | 3.5 | 0.0 | 0.0 | 0.0 | 0.0 | 0.5 | 5.0 | 12.0 | 14.5 |
| Operating cost | | | | | | | | | | | | | | | | |
| Plants and storage facilities ($10^3$ \$ per day) | 50 | 245 | 496 | 676 | 22 | 112 | 232 | 324 | 3 | 22 | 49 | 71 | 50 | 271 | 550 | 785 |
| Transportation modes ($10^3$ \$ per day) | 0 | 2 | 7 | 11 | 0 | 0 | 2 | 3 | 0 | 0 | 0 | 0 | 0 | 6 | 12 | 17 |
| Total daily cost ($10^3$ \$ per day) | 127.67 | 496.63 | 549.28 | 726.58 | 66.20 | 240.58 | 271.15 | 344.59 | 42.62 | 39.40 | 67.33 | 83.19 | 191.50 | 483.69 | 692.51 | 860.60 |
| Cost per kg $H_2$ (\$) | 16.17 | 8.36 | 3.96 | 3.67 | 16.73 | 8.10 | 3.91 | 3.48 | 53.74 | 6.63 | 4.85 | 4.20 | 12.76 | 4.28 | 2.63 | 2.29 |

the demand is. Based on this conclusion, the UPC calculation could be improved in order to take into account different costs for electrolysis process resulting from different energy sources and technologies (wind, PV, hydro…). For that, a new calculation approach of the UPC is needed and will be implemented in our further works.

In the original model, the UPC is a fixed parameter which only varies depending on the size of the production unit but does not integrate the contribution of the different costs leading to the unit production cost ($ per kg $H_2$). Yet, as mentioned in the (McKinsey&Company 2010) report, a better vision of UPC is to consider the fixed, electricity, and feedstock costs. The fixed cost is related to labor and maintenance. For the sake of illustration, a value of electricity consumption of 0.48 $kWh_{elec}$/kg $H_2$ for the small and medium central plants of SMR and 0.44 $kWh_{elec}$/kg $H_2$ for larger plants in 2020 is predicted (McKinsey&Company 2010). All the contributions are reflected in Eq. (5), where the UPC calculation ($ per kg $H_2$) is given by the addition of the fixed cost of a production plant type p size j in the time period $t$ ($FCP_{epjt}$, $ per kg $H_2$), the electricity cost for general usage in a production plant type p size j projected for the time period $t$ ($EC_{epjt}$, $ per kg $H_2$) and the feedstock e cost for production plant p type size j ($FSC_{epjt}$). The $FSC_{epjt}$ is obtained by multiplying the feedstock $e$ efficiency in the process $p$ size $j$ in time $t$ ($kWh_{elec}$/kg $H_2$) by the feedstock $e$ price ($/$kWh_{elec}$), for electrolysis process, the feedstock is considered as electricity and the energy source cost will vary depending on the type, e.g., fossil vs. renewable (see Supplementary Material, Table 6).

$$UPC_{e,p,j,t} = FCP_{e,p,j,t} + EC_{e,p,j,t} + FSC_{e,p,j,t} \tag{5}$$

The feedstock cost is likely to gain importance because it depends on the energy transition scenario and could induce a cost change of renewable energy impacting the hydrogen cost in the long time horizon from 2020 to 2050.

– According to the results, the demand and CCF have the greatest impact in the TDC but PCC is also important. The other parameters have some impact, but only through their interaction.
– By taking into account the parameters and the uncertainty (e.g., the demand), the objective function of the HSC can be improved by considering a more realistic representation as the net present value (NPV) for decreasing the current CCF impact in the optimization results. Efforts to represent and integrate demand uncertainty are also mandatory. Finally, some efforts to better represent capital costs of facilities can take place as well as the new calculation of UPC.

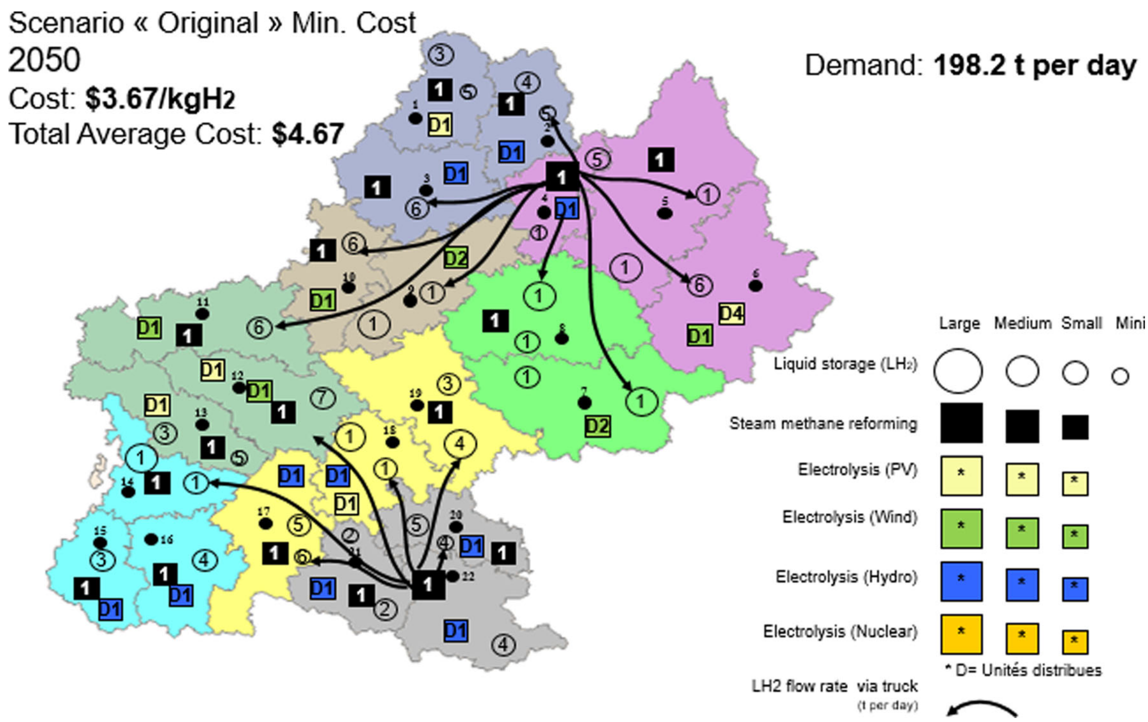


Fig. 5 Map of the original scenario in 2050

Various experiments have been performed and have highlighted that the main interactions are as follows: demand × CCF, demand × UPC, demand × CCF × UPC, and demand × CCF × SCC.

## Conclusions and Perspectives

In this paper, a sensitivity analysis (SA) is performed in the logistic model of the HSC to detect the most sensitive

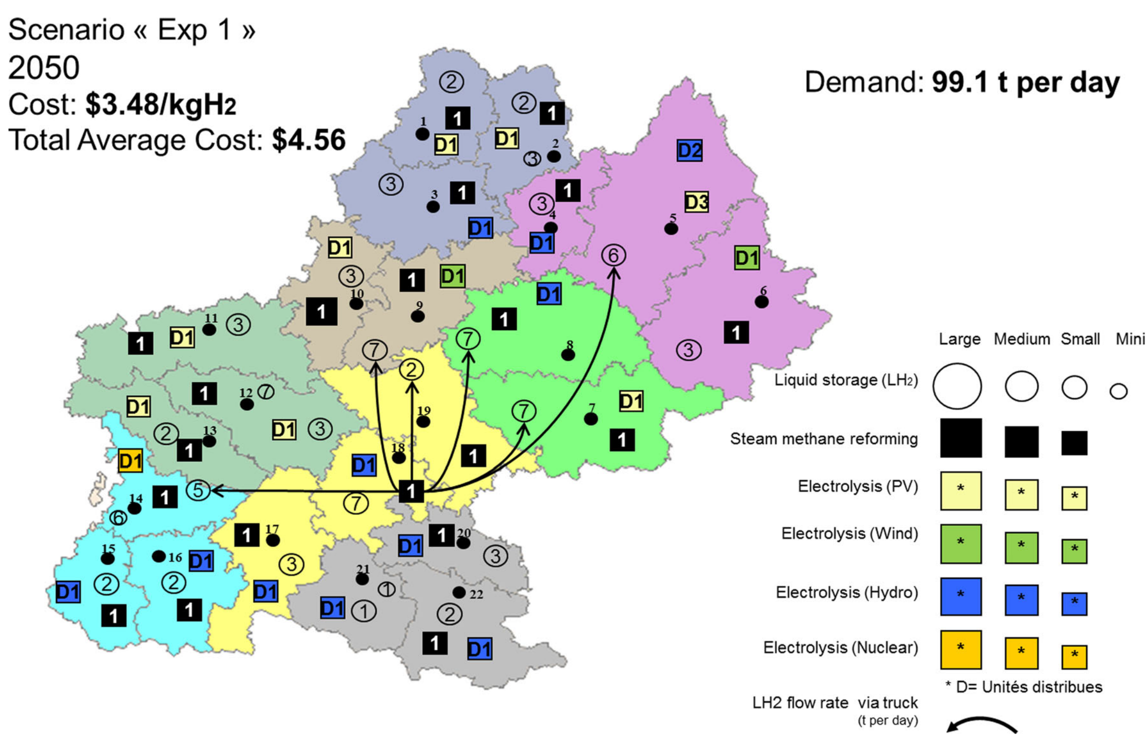


Fig. 6 Map of the scenario “Exp 1” in 2050

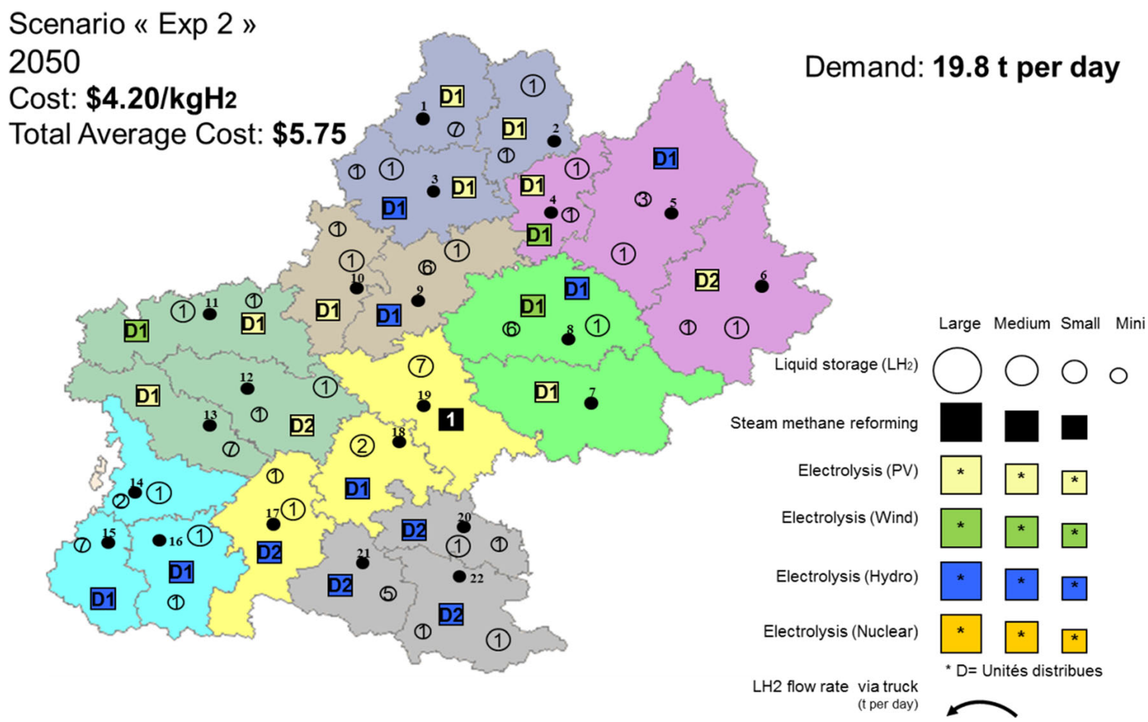


**Fig. 7** Map of the scenario "Exp 2" in 2050

parameters and their interactions. Six important factors were analyzed: demand, capital change factor (CCF), storage and production capital costs (SSC and PCC), learning rate (LR), and unit product cost (UPC). A special attention has been paid on the response variable, i.e., the total daily cost (*TDC*). The chosen methodology to perform the SA was the DOE through the use of statistical tools such as factorial design and response surface methods. This methodology is considered to be more consistent than the one-at-a-time approach mainly for two reasons: first, quantitative results are generated in a few optimization runs and the method has the advantage to measure parameter interactions. The implementation of these statistical

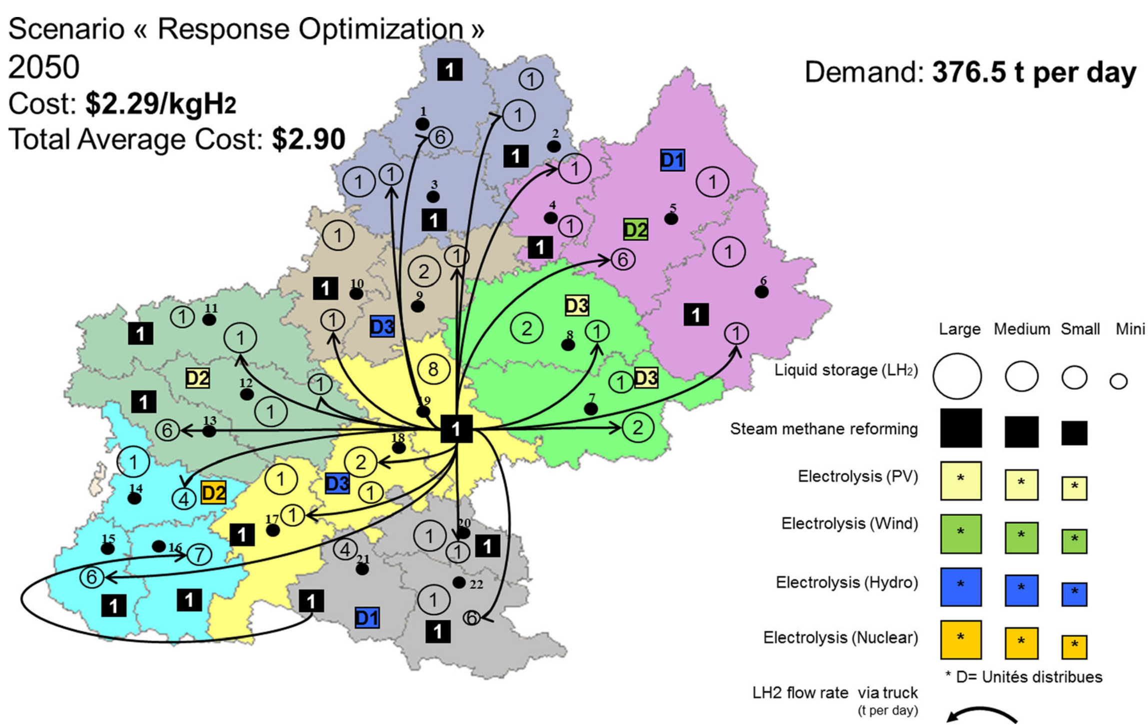


**Fig. 8** Map of the scenario "Optimization response" in 2050

methods for the SA of the HSC is one of the main contributions of this paper. The SA was grouped into two experiments (one linear and one quadratic). In both experiments, not surprisingly, the demand is the factor that is by far the most significant parameter that strongly conditions the optimization criterion of the original HSC model, the second most important parameter is the capital change factor. Then, any change that could occur relative to demand or CCF could strongly affect the variable response.

As the demand is a very important parameter, special attention must be paid to its modeling. One of the characteristics in the future HSCs is the fact that the demand is not yet known. For that, its uncertainty is an important issue to be taken into account. Several strategies could thus be implemented to tackle demand uncertainty, implementing DOE for each one to analyze its impact in the objective function.

Concerning the other factors, PCC and, in a less extent, LR are also important. The main interactions are between demand, CCF, UPC, and SCC, founding so that the calculation of UPC must be improved. The set of the best levels of experiments 1 and 2 and the optimization run are compared with those previously obtained for Midi-Pyrénées with cost minimization. No significant difference is observed between the original model and experiment 1. Experiment 2 presents a difference mainly in the first period and in the transport between grids, mostly due to the low value of the demand. For the optimization response, a significant difference is observed, mainly in the hydrogen cost per kilogram.

Some perspectives of this work can be highlighted. Based on the results regarding the *CCF*, the calculation of the *TDC* could be improved by the use of discounted costs associated with each time period (Sabio et al. 2010) to be less influenced by the CCF and the *LR* parameters. The NPV profitability criterion could also be used as an objective function. Subventions could also be taken into account to help and initiate the HSC. A sensitivity analysis of some elements of the operational costs (e.g., the rate of utilization of primary energy source or the process efficiency) could also be performed as well as the analysis of a high variation in energy source availability. Some previous studies have already considered some of these factors (ADEME 2015; Burrill 1997). Other parameters such as the safety stock period, new tube trailer capacities, and the use of pipelines could also be evaluated in future case studies. Considering that the most important parameter is the demand, more effort is needed to find the more consistent way to model this parameter especially since a long time horizon is considered. It must be emphasized that demand uncertainty has been introduced before by Almansoori and Shah (2012) and Kim et al. (2008) through scenario analysis. Although uncertainty could be considered as a mature area (Fahimnia et al. 2015), optimization models that incorporate it are usually large in size and difficult to solve (Papageorgiou 2009; Snyder et al. 2014; Garcia and You 2015) so that algorithmic and computational challenges still arise to address uncertainty modeling techniques.

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