Anton Ochoa Bique*, Leonardo K. K. Maia, Ignacio E. Grossmann and Edwin Zondervan

Design of hydrogen supply chains under demand uncertainty – a case study of passenger transport in Germany

Abstract: A strategy for the design of a hydrogen supply chain (HSC) network in Germany incorporating the uncertainty in the hydrogen demand is proposed. Based on univariate sensitivity analysis, uncertainty in hydrogen demand has a very strong impact on the overall system costs. Therefore we consider a scenario tree for a stochastic mixed integer linear programming model that incorporates the uncertainty in the hydrogen demand. The model consists of two configurations, which are analyzed and compared to each other according to production types: water electrolysis versus steam methane reforming. Each configuration has a cost minimization target. The concept of value of stochastic solution (VSS) is used to evaluate the stochastic optimization results and compare them to their deterministic counterpart. The VSS of each configuration shows significant benefits of a stochastic optimization approach for the model presented in this study, corresponding up to 26% of infrastructure investments savings.

Keywords: fuel infrastructures; hydrogen supply chain design; mixed integer linear programming; stochastic optimization; water electrolysis technology.

1 Introduction

The population is constantly growing and consuming more energy year after year [1, 2]. The transportation sector plays a crucial role in human life and faces major challenges concerning sustainability. Up until now, fossil fuels are the primary energy sources for the transportation sector, which is the second largest contributor of carbon dioxide emissions worldwide. The transportation sector faces an increase in energy demand.

***Corresponding author: Anton Ochoa Bique**, Department of Production Engineering, Laboratory of Process Systems Engineering, Universität Bremen, Leobener Str. 6, 28359 Bremen, Germany, E-mail: anthonob@gmail.com. https://orcid.org/0000-0003-1154-0603
Leonardo K. K. Maia, Department of Production Engineering, Laboratory of Process Systems Engineering, Universität Bremen, Leobener Str. 6, 28359 Bremen, Germany
Ignacio E. Grossmann, Department of Chemical Engineering, Carnegie Mellon University, Doherty Hall, 5000 Forbes Ave, Pittsburgh, PA 15213, USA
Edwin Zondervan, Faculty of Science and Technology, University of Twente, De Horst 2, 7522 LW Enschede, The Netherlands

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For example, in Germany the transportation sector's share of final energy demand has increased from 26.1% in 1990 to 29.8% in 2015 [3]. The increasing energy demand and the current issues on sustainability have been driving the efforts to replace current sources of energy by more efficient ones such as solar, wind and/or biomass [4, 5]. The vehicle industry has been working on the improvement of fuel efficiency considering the use of electricity and on low carbon energy-efficient transport via renewable energy sources such as biodiesel and methanol. Nowadays, battery electrical vehicles (BEV) and fuel cell electrical vehicles (FCEV) are two promising options for a new type of green transportation system. However, such changes will require a new infrastructure and a smart transition strategy to turn the transportation sector into a carbon-free system. Analysis of large-scale integration of these vehicles technologies have shown competitive advantages of FCEVs [6–8]. Hydrogen is one of the most efficient fuels (2.5 times more efficient than gasoline in terms of energy density) and can be obtained both from renewable and from non-renewable sources. However, the main challenge to make the use of hydrogen in vehicles feasible is to build a completely new hydrogen generation network considering an investment in large-scale FCEV production and high FCEV demand uncertainty [9]. It stands behind the development of a hydrogen supply chain (HSC) considering safety, economic and environmental impact issues [10].

Many studies in the area of HSC design focus on network evaluation using steady-state simulation [3, 11, 12]. The work of Hugo et al. considers all possible hydrogen alternatives for an optimal hydrogen infrastructure design [13]. Kim and Moon consider a bi-criterion assessment of a HSC network. The model they propose determines cost-safety objectives, where the safety objective is based on the so-called risk index method [14]. De-León Almaraz et al. propose a design of a HSC considering three objectives: cost, environmental impact and risk. It is solved by the ε-constraint method [15]. Several contributions by Almansoori et al. investigate a number of strategic decisions to design HSC networks in Germany and Great Britain at large-scale considering emission targets and carbon taxes as a part of the model formulation [16, 17]. The studies focus on satisfaction of hydrogen demand, which was determined by a 10% implementation of FCEVs into the passenger transport system. The studies of Lahnaoui et al. and Reuß et al. focus on the development of cost-effective HSC network based on excess electricity from wind energy by 2050. It shows potential of FCEVs penetration into transportation sector [3, 7].

However, it is recognized that input data is uncertain in most real-world decision problems and has a major effect on decisions in supply chain. Uncertainty can be identified as one of the major challenges in supply chain management [18, 19]. The work of Kim et al. extended their earlier mathematical formulation considering demand uncertainty following a stochastic formulation based on a two-stage programing approach. The model was applied to evaluate the HSC of Korea [20]. The work of Almasoori and Shah takes into account uncertainty in hydrogen demand over a long-term planning horizon using a scenario-based approach. A multi-stage stochastic mixed integer linear programming (MILP) model was proposed to determine possible configurations of HSC network in Great Britain [21].

In previous works, it is noted that renewable energy as a power source has the potential to replace commonly used fossil fuels in the near future: renewable-based electricity production will be enough to satisfy personal needs such as household's energy demand and hydrogen based fuel demand [22]. Moreover, the best trade-off solution of multi-objective optimizations shows significant dominance of water electrolysis technology against the rest [23]. This work is an extension of a previous model [22] developed by the authors to capture hydrogen demand uncertainty, where environmental impact is part of a cost network assessment, and penalty method is applied to analyze the economic value of supply security. In this work, a model of the HSC network is developed for the transportation sector in Germany considering a significant FCEVs penetration into the consumer market to show the potential of a hydrogen infrastructure. The proposed stochastic model is a Mixed-integer Linear Program that is solved in AIMMS/CPLEX.

2 Sensitivity analysis

There are many problems in production planning and scheduling, location and transportation design requiring decisions to be made in the presence of uncertainty [24]. It is not easy to identify which parameters in the model are random. Moreover, optimization under uncertainty leads to very large-scale optimization models. Thus, it is important to control the size of the model by only taking into account the uncertain parameters that have the largest impact. Uncertainty can be classified as presented in Table 1, where the first three classes are considered most often in supply chain management [25]:

Supplier failure and Supplier insolvency are a source for uncertainties, which means the inability to handle demand fluctuations and quality problems at supplier plants.

Table 1: Classification of uncertainty.

Location in the process	Classification of uncertainty sources
SUPPLY	Supplier failure; supplier insolvency
PROCESS	Delays; delivery constrains; production resources disturbances; production system input disturbances
DEMAND	Purchasing power; competitors
EXTERNAL	Outsourcing of production; behavioral, political and social disruptions

Process uncertainties cover all risks associated with internal operations: delays caused by supply disruptions or problems in unloading and loading; the breakdown of machines (production resource disturbance); financial factors (production system input disturbance).

In the literature, attention has been paid to modeling of systems under demand uncertainty [14, 21, 26]. The demand quantity results in missed income, in case of under production, or high production and stocking costs (over production). Moreover, competitors can either produce a similar product or use a new approach for an existing product, which have an effect on product demand. In addition, the demand can decrease if the purchasing power decreases.

The last class of uncertainty sources includes outsourcing, behavioral, political and social, and disruptions sources. Outsourcing is associated with intellectual property risks (the risk of unlicensed production). Behavioral uncertainties arise from the lack of information sharing between different echelons in the supply chain such as retailers and suppliers. Political and social uncertainties cover laws and policies, social acceptance. Uncertainty of disruptions relates to the war, terrorism, natural disasters, and infrastructure risks.

Therefore, it is important to identify which parameters in the model are uncertain. For this, a local sensitivity analysis is performed to evaluate which model parameters have the strongest impact on the objective function and the decision variables. From the aforementioned uncertainty sources, several parameters can be analyzed:
- the price of raw materials (supply uncertainty);
- operational problems in unloading and loading (process uncertainty);
- demand quantity (demand uncertainty);
- carbon tax (external uncertainty).

Each of the selected parameters is evaluated within a ±20% range from their base values and applied in the deterministic model. Figure 1 shows the sensitivities of all

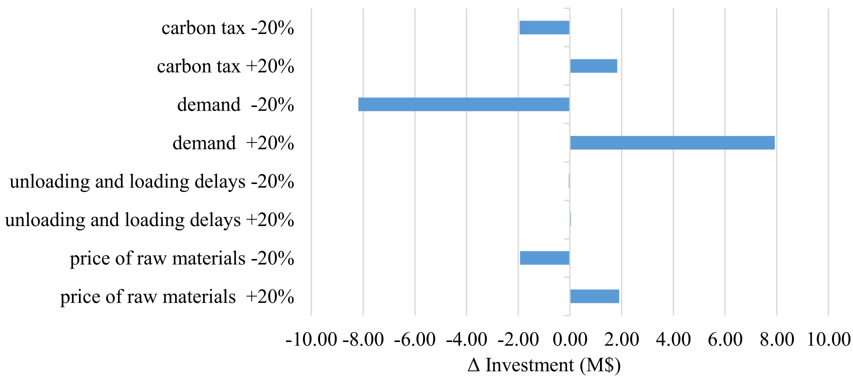

Figure 1: Sensitivities of selected parameters on objective function (total daily cost).

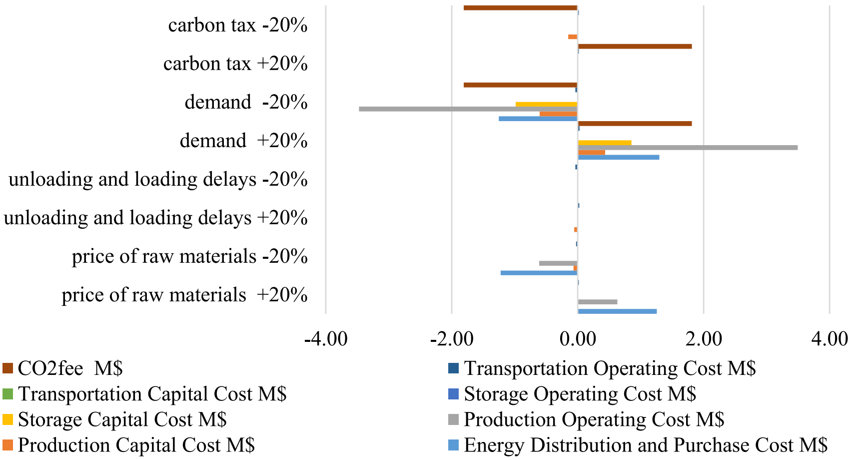

Figure 2: Sensitivities of selected parameters on other decision variables in the model.

selected parameters on the objective function, while Figure 2 shows the sensitivities on the remaining decision variables of the model. It is clear that hydrogen demand has the greatest effect on the objective function compared to other parameters. Thus, demand is considered as the uncertain parameter in the stochastic formulation.

3 Network description and problem statement

The analysis of previous studies [22, 23] shows that the combination of water electrolysis and steam methane reforming technologies can satisfy the hydrogen demand for trade-offs between costs, environmental impact and safety of the network. This study considers two configurations of a HSC, which are analyzed and compared to each other according to production types: water electrolysis versus steam methane reforming. Each configuration represents the design of a HSC network for Germany up to 2050 and has cost minimization as the target. The two configurations are summarized as follows:

Configuration 1: Hydrogen can be produced in small-, medium-, and large-scale plants via steam methane reforming (SMR) (see Section 3.2.3). Hydrogen distribution takes place in two forms from production to storage sites via railway tank car and tanker truck (liquid hydrogen), and railway tube car and tube trailer (gaseous hydrogen). There are two types of storage technology (super-insulated spherical tank, and pressurized cylindrical vessels). The uncertainty of the hydrogen demand is presented as a multi-stage stochastic optimization problem with three demand scenarios, referred to as “high” (+20% expected demand), “medium” (expected demand), “low” (–20% expected demand) scenarios over five time periods of planning horizon, with corresponding probabilities at 0.3, 0.4, 0.3, respectively.

Configuration 2: Similar to the first configuration, we consider water electrolysis (WE) as a hydrogen production technology.

3.1 Problem description

Given are the location and capacity of energy source suppliers, the capital and operating costs for transportation modes, the hydrogen production and storage facilities for a particular size and their global warming potential indicator, assuming:

1. the locations of storage facilities are fixed;
2. electricity is the main energy source to power rail freight transport;
3. the electricity price is based on the industrial price for Germany;
4. the handling of residual waste is neglected;
5. secondary energy carriers have no economic value in this network model;
6. electricity costs are the same everywhere without any transmission bottlenecks (the German copper plate power grid assumption).

The HSC consists of three types of energy sources from different origins: wind and solar energy, natural gas; two types of large-scale hydrogen production technologies: steam methane reforming, water electrolysis; two types of product form: gaseous, liquid; four types of transportation modes, where two of them are used to distribute each product form: liquid – railway tank car, tanker truck, gaseous – railway tube car, tube trailer; two types of storage technologies: super-insulated spherical tank, pressurized cylindrical vessels (see Figure 3).

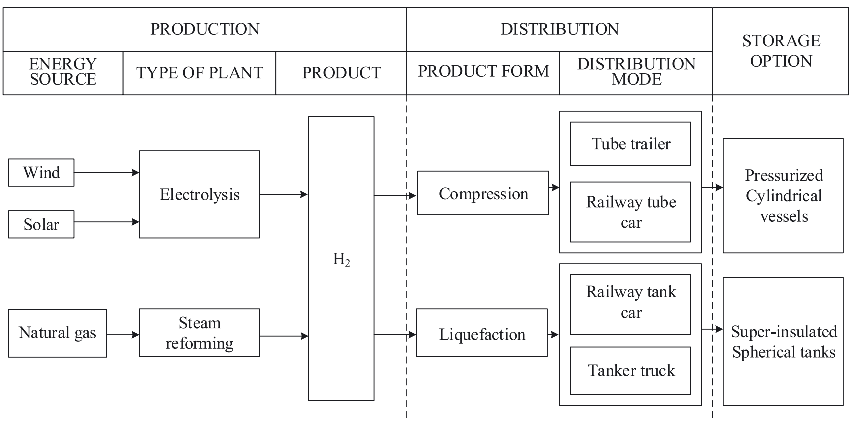

Figure 3: Structure of the hydrogen supply and delivery chain.

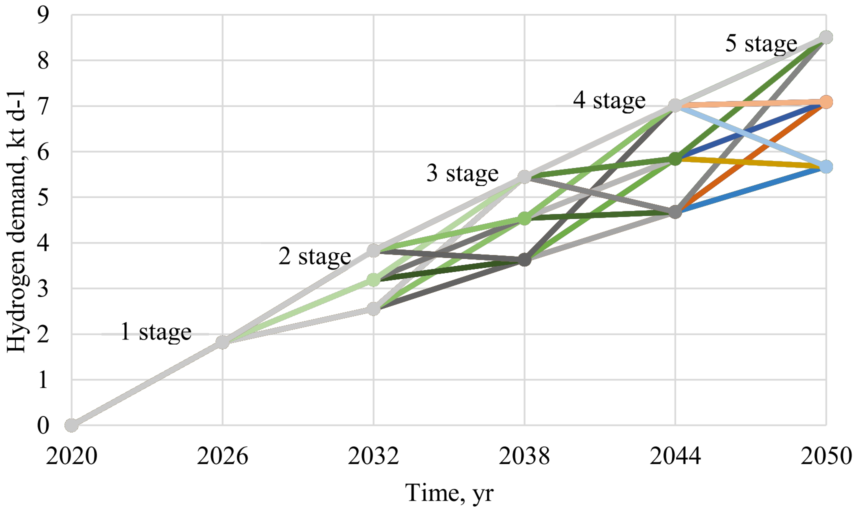

Figure 4: Demand scenario tree (trajectory).

Each facility in the HSC includes a technological option, a capacity, and a location. Each scenario includes a number of decisions that have to be taken. This work considers multi-stage stochastic MILP model representations including five time periods and 81 scenarios. Each time period represents a six-year interval starting from 2020 until 2050 (see Figure 4).

Each scenario has a uniquely defined demand value as shown Figure 5. It is assumed that the demand is known at the first-stage, while at the next stages different corrective actions are taken according to unique demand values of all scenarios. The tree structure is formulated using non-anticipativity constraints [27] that do not allow the solution to anticipate on stochastic outcomes that lie beyond the stage. The problem is concerned with finding the size, capacity and locations of the production facilities for an uncertain demand, so as to minimize the cost of the first-stage and the expected cost of the following stages. To analyze the economic value of supply security, a cost penalty for demand that is not satisfied is applied. The main idea of penalty functions is to apply a penalty to feasible solutions when the constraint of the hydrogen demand requirements is violated [28]. To evaluate the stochastic optimization results and compare them to their deterministic counterpart the concepts of expected value of perfect information (EVPI) and value of stochastic solution (VSS) are used, where the EVPI measures the value of having accurate information for the future demand while the VSS assesses the value of cost when ignoring uncertainty in the demand [29].

The data was collected from the Federal Statistical Office of Germany [30], the Fraunhofer Institute for Solar Energy Systems ISE [31], Almansoori and Betancourt-Torcat [17], Ruth [32].

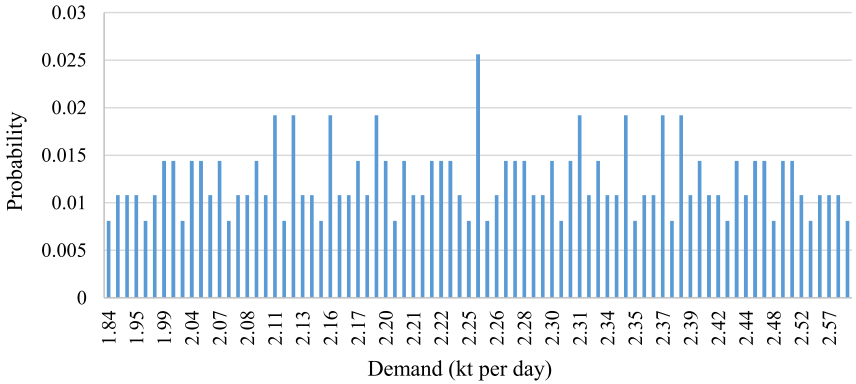

Figure 5: Demand distribution. Values shown correspond to total demand for each scenario up to 2050.

3.2 Formulation of the HSC

In Figure 6 the superstructure of the HSC model is show. The superstructure includes all the possible connections between the model components. It consists of six main components: grid points g (each grid point represents a German state), energy sources e, different transportation modes t, different hydrogen production- p and storage facilities s, hydrogen produced forms f. In the following subsections, each component of the HSC model is described in more detail [23].

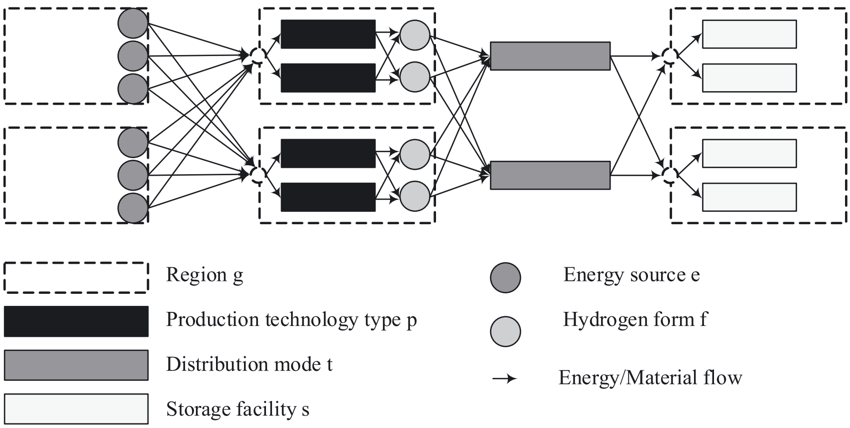

Figure 6: Model superstructure.

3.2.1 Grid

The landscape of Germany is divided into 16 grid points representing German regions. The hydrogen production and storage facilities should be located at the region's largest city to satisfy the local demand and to further distribute the products.

3.2.2 Primary energy sources

The primary energy resource availability at each grid point is used to define the type, size and location of production technologies. Additionally, the main problem of a domestic production facility is related with the energy source consumption from, i) a domestic grid point, or ii) supply from neighboring grid points, or iii) import from abroad.

3.2.3 Hydrogen production and demand

Four types of technologies to produce hydrogen were included in model: steam methane reforming, coal gasification, biomass gasification and water electrolysis. Each facility has fixed capital- and operational costs. The main decisions to be made are: the type, capacity and location of production facilities. Each production technology is coupled with an index *h* for different capacities, referred to as small (up to 10 $t\ H_2\ d^{-1}$), medium (up to 150 $t\ H_2\ d^{-1}$), and large (up to 480 $t\ H_2\ d^{-1}$). The total hydrogen demand was estimated based on the FCEVs penetration rate into the total number of passenger transports (public buses, light motor vehicle) available by chosen time period *ts*.

3.2.4 Hydrogen physical form

Hydrogen can be carried in two physical forms: liquid and gaseous. The selection of the form helps to define the type of transportation mode and which storage facility should be used in the HSC. These decisions affect the final costs of the HSC network.

3.2.5 Transportation mode

The transportation mode is related to the selected form of produced hydrogen. The main decision is to select the transportation mode and the number of vehicles used to deliver the final product from production site to storage site. Each transportation mode has a specific capacity, capital cost, operating cost. It should be noted that the operating cost is associated with the delivery distance (including fuel, labor, maintenance and general expenses).

3.2.6 Storage facility

The storage facility is linked to the hydrogen form as well as to the transportation mode. The main decision is to select the number of a certain type of storage facilities that should be installed to store the final product for 10 days. Each type has a specific capacity (540 $t\,H_2\,d^{-1}$), capital and operating cost. Storage facilities are installed at each grid point to satisfy the local hydrogen demand. It is noted that these facilities can be located on- or off site.

4 Mathematical formulation

The objective is to minimize the total cost of the HSC network. The multistage stochastic linear program is to find the size, capacity and locations of the production facilities for an uncertain demand, considering the minimum cost of the first-stage and the expected cost of the next stages as follows:

$$\min c^1x^1 + E_\Omega\left[c^2x^2 + \ldots + c^Hx^H\right] s.t. W^1 \cdot x^1 = h^1, T^{ts-1} \cdot x^{ts-1} + W^{ts} \cdot x^{ts} = h^{ts}, ts = 2, \ldots, H, x^1 \geq 0, x^{ts} \geq 0,\ ts = 2, \ldots, H; \tag{1}$$

where c – first-stage objective $c^{ts}x$, E – mathematical expectation operator, left-hand side vector of an optimality cut in the L-shaped method, or an event, h – right-hand side vector in stage (time period) ts ($W^{ts} \cdot x^{ts} = h^{ts} - T^{ts-1} \cdot x^{ts-1}$, where $W^{ts}x^{ts}$ compensates for a possible inconsistency of the system $T^{ts-1}x^{ts-1} \leq h^{ts}$), H – number of stages (horizon) in multistage problems. x – first-stage decision vector or multistage decision vector x^{ts}, W – recourse matrix, T – technology matrix, Ω – set of all random events.

In the following subsections the model constraints and objective function are described in more detail.

4.1 Constraints

4.1.1 Demand constraints for a certain energy source

The demand for a certain energy source must be satisfied to ensure production. The demand for a certain energy source is calculated as follows:

$$\mathrm{ESD}_{sc,ts,g,p,e} = \sum_{f,h} \mathrm{HP}_{sc,ts,g,p,h,f} \cdot \alpha_{e,p,h}, \forall e, p, g, ts, sc \tag{2}$$

where $\mathrm{HP}_{sc,ts,g,p,h,f}$ denotes the amount of produced hydrogen in the production facility p size h in the form f at the grid point g during time period ts for scenario sc. The parameter $\alpha_{e,p,h}$ denotes the ratio between the energy sources e consumption to produce 1 kg of hydrogen in production facility p size h. As mentioned before, the main problem of a domestic production facility is concerned with finding an appropriate energy source supplier. The demand must be covered by one or a combination of the following: local power generation, imports from neighboring grid points or import from abroad.

$$\mathrm{ESD}_{sc,ts,g,p,e} \le \sum_{g''} \mathrm{PESAv}_{sc,ts,g'',g,p,e} + \mathrm{PESIm}_{sc,ts,g,p,e}, \forall e,p,g,ts,sc \tag{3}$$

In (3) $\mathrm{PESAv}_{sc,ts,g'',g,p,e}$ is the energy source flowrate to meet demand for a certain energy source e in production facility p from the grid point g'' to the grid point g during time period ts for scenario sc, $\mathrm{PESIm}_{sc,ts,g,p,e}$ is the flowrate importing energy source e to the grid point g, where production facility p is installed, during time period ts for scenario sc. Moreover, the energy source flowrate is limited by the feedstock availability in grid points as follows:

$$\sum_{g} \mathrm{PESAv}_{sc,ts,g'',g,p,e} \le \mathrm{ESAv}_{ts,g'',e}, \forall e,p,g'',ts,sc \tag{4}$$

where $\mathrm{ESAv}_{ts,g'',e}$ is the amount of available energy source e at grid point g at time period ts.

4.1.2 Hydrogen demand constraints

The total hydrogen demand projections were calculated based on work presented by Lahnaoui et al. [3]. The hydrogen demand by grid point can be calculated as follows:

$$\mathrm{HD}_{sc,ts,g} = \gamma_{ts}\mathrm{PN}_{sc,ts,g} \cdot \mathrm{AvD}_{ts} \cdot \mathrm{FE}, \forall g,ts,sc \tag{5}$$

where γ_{ts} represents the FCEVs penetration rate in time period ts, $PN_{sc,ts,g}$ is population size at grid point g in time period ts for scenario sc, AvD_{ts} is the average distance travelled by a person at time period ts, and FE denotes the fuel economy. The demand must be satisfied by the network and/or imports from another country:

$$\mathrm{HD}_{sc,ts,g} \le \sum_{f} \left(\mathrm{HD}_{sc,ts,g,f} + \mathrm{HI}_{sc,ts,g,f}\right), \forall g,ts,sc \tag{6}$$

$\mathrm{HD}_{sc,ts,g,f}$ represents the fraction of the hydrogen demand fulfilled by the network in the form f in grid point g at time period ts and scenario sc, $\mathrm{HI}_{sc,ts,g,f}$ represents the fraction of hydrogen imported from another country in form f at grid point g at time period ts and scenario sc. The hydrogen demand in the form f must be satisfied by local production and/or from neighboring grid points:

$$\mathrm{HD}_{sc,ts,g,f} \le \sum_{t,g'} \mathrm{HF}_{sc,ts,g',g,t,f}, \forall f,g,ts,sc \tag{7}$$

where $\mathrm{HF}_{sc,ts,g',g,t,f}$ is the hydrogen flow in the form f from grid point g' to g via transportation mode t during time period ts for scenario sc.

4.1.3 Hydrogen generation constraints

The hydrogen production is described as:

$$\mathrm{HP}_{sc,ts,g,f} = \sum_{p,h} \mathrm{HP}_{sc,ts,g,p,h,f}, \forall g, f, ts, sc \tag{8}$$

where $\mathrm{HP}_{sc,ts,g,f}$ represents the hydrogen generation in form *f* at grid point *g* during time period *ts* for scenario *sc*, $\mathrm{HP}_{sc,ts,g,p,h,f}$ represents of the quantity of hydrogen produced in facility *p with* size *h* in the form *f* at grid point *g* during time period *ts* for scenario *sc*.

The hydrogen production rate is constrained by minimum and maximum capacities as:

$$\mathrm{MinPCap}_{p,h} \cdot \mathrm{NPF}_{ts,g,p,h,f} \le \mathrm{HP}_{sc,ts,g,p,h,f} \le \mathrm{MaxPCap}_{p,h} \cdot \mathrm{NPF}_{ts,g,p,h,f}, \forall g, p, f, ts, sc \tag{9}$$

where $\mathrm{MinPCap}_{p,h}$, $\mathrm{MaxPCap}_{p,h}$ is the min/max production capacity for hydrogen production facility *p* size *h*, $\mathrm{NPF}_{ts,g,p,f}$ represents the number of installed production plants *p* size *h* at grid point *g* at time period *ts*.

4.1.4 Hydrogen distribution constraints

The hydrogen flow in form *f* from grid point *g* to grid point *g′* will exist if the transportation mode *t* has been selected:

$$\mathrm{MinHF}_{t,f} \cdot X_{sc,ts,g,g',t,f} \le \mathrm{HF}_{sc,ts,g,g',t,f} \le \mathrm{MaxHF}_{t,f} \cdot X_{sc,ts,g,g',t,f}, \forall sc, ts, g, g', t, f \tag{10}$$

where $\mathrm{MinHF}_{t,f}$, $\mathrm{MaxHF}_{t,f}$ are min/max product flow rate, $X_{sc,ts,g,g',t,f}$ is a binary variable, which equals 1 if product transportation in form *f* from grid point *g* to grid point *g′* by transportation mode *t* is established during time period *ts* for scenario *sc*. It should be noted that products can be imported to a particular grid point from neighboring grid points or be exported to other grid points in one direction:

$$Q_{sc,ts,g,f} \ge X_{sc,ts,g,g',t,f}, \forall sc, ts, g, g', t, f : g <> g' \tag{11}$$

$$W_{sc,ts,g,f} \ge X_{sc,ts,g',g,t,f}, \forall sc, ts, g, g', t, f : g <> g' \tag{12}$$

$$W_{sc,ts,g,f} + Q_{sc,ts,g,f} \le 1, \forall sc, ts, g, f \tag{13}$$

where $Q_{g,f}$, $W_{g,f}$ are binary variables, which are equal 1 if product in form *f* is exported/imported respectively. The product flowrate by transportation mode *t* from *g* to *g′* during time period *ts* for scenario *sc* is given as:

$$\mathrm{HP}_{sc,ts,g,f} \ge \sum_{t,g'} \mathrm{HF}_{sc,ts,g,g',t,f}, \forall g, f, ts, sc \tag{14}$$

The number of vehicles *t* required in grid point *g* to serve local and regional demand of hydrogen produced in the form *f* during time period *ts* is given as follows:

$$\mathrm{NTU}_{ts,g,g',t,f} \geq \frac{\mathrm{HF}_{sc,ts,g,g',t,f}\left(\frac{2\mathrm{Dis}_{g,g',t}}{\mathrm{AvS}_t} + \mathrm{LUT}_t\right)}{\mathrm{MA}_t \cdot \mathrm{TCap}_{t,f}} + \mathrm{ExT}_{sc,ts,g,g',t,f}, \forall_{sc,ts,g,g',t,f} \tag{15}$$

where $\mathrm{Dis}_{g,g',t}$ is the average distance travelled by transportation unit t to serve local and regional demand, AvS_t is the average speed of transportation unit t, LUT_t is the load/unload time for transportation unit t, MA_t is transportation unit t availability, $\mathrm{TCap}_{t,f}$ is capacity of transportation unit t to distribute produced hydrogen in form f, $\mathrm{ExT}_{sc,ts,g,g',t,f}$ is continuous variable in scenario sc with value between 0 and 1, which is used to take an integer value for $\mathrm{NTU}_{ts,g,g',t,f}$ (modification was suggested by De-León Almaraz et al. [15]).

4.1.5 Hydrogen storage constraints

The required hydrogen storage is constrained by maximum and minimum capacities as:

$$\mathrm{MinSCap}_{s,f} \cdot \mathrm{NSF}_{ts,g,s,f} \leq \mathrm{HSInv}_{sc,ts,g,s,f} \leq \mathrm{MaxSCap}_{s,f} \cdot \mathrm{NSF}_{ts,g,s,f}, \forall g,s,f,ts,sc \tag{16}$$

where $\mathrm{NSF}_{ts,g,s,f}$ denotes the number of storage facilities s holding hydrogen in form f at grid point g during time period ts, and $\mathrm{MinSCap}_{s,f}$, $\mathrm{MaxSCap}_{s,f}$ represent the minimum and maximum capacities of storage facility s for holding hydrogen in the from f, $\mathrm{HSInv}_{sc,ts,g,s,f}$ is inventory of product f in the storage facility s at grid point g at time period ts and scenario sc.

The hydrogen inventory level at the storage facility is described by,

$$\sum_s \mathrm{HSInv}_{sc,ts,g,s,f} \geq \tau \cdot \mathrm{HD}_{sc,ts,g,f}, \forall f,g,ts,sc \tag{17}$$

where τ is total product storage period.

4.1.6 Time evolution constraints

As the network evolves over time, the number of production and storage facilities, and transportation units at current time period equals the number of invested units at previous time step plus the number of new invested facilities meet the increased demand. This can be described as using the following constraints:

$$\mathrm{NPF}_{ts,g,p,h,f} = \mathrm{NPF}_{(ts-1),g,p,h,f} + \mathrm{InPF}_{ts,g,p,h,f}, \forall ts,g,p,h,f : ts \neq ts1 \tag{18}$$

$$\mathrm{NSF}_{ts,g,s,f} = \mathrm{NSF}_{(ts-1),g,s,f} + \mathrm{InSF}_{ts,g,s,f}, \forall ts,g,s,f : ts \neq ts1 \tag{19}$$

$$\mathrm{InTU}_{ts,g,t,f} = \sum_{g'} \mathrm{NTU}_{ts,g,g',t,f} - \sum_{g'} \mathrm{NTU}_{(ts-1),g,g',t,f}, \forall ts,g,t,f : ts \neq ts1 \tag{20}$$

where $\mathrm{InPF}_{ts,g,p,h,f}$, $\mathrm{InSF}_{ts,g,s,f}$ and $\mathrm{InTU}_{ts,g,t,f}$ are the number of new invested production and storage facilities, and transportation units, respectively at grid point g.

During the first period, the number of production and storage facilities, and transportation units are given by,

$$\mathrm{NPF}_{ts1,g,p,h,f} = \mathrm{ExNPF}_{g,p,h,f} + \mathrm{InPF}_{ts1,g,p,h,f}, \forall g,p,h,f \tag{21}$$

$$\mathrm{NSF}_{ts1,g,s,f} = \mathrm{ExNSF}_{g,s,f} + \mathrm{InSF}_{ts1,g,s,f}, \forall g,s,f \tag{22}$$

$$\mathrm{InTU}_{ts1,g,t,f} = \sum_{g'} \mathrm{NTU}_{ts1,g,g',t,f} - \mathrm{ExTU}_{g,t,f}, \forall g,t,f \tag{23}$$

where $\mathrm{ExNPF}_{g,p,h,f}$, $\mathrm{ExNSF}_{g,s,f}$ and $\mathrm{ExTU}_{g,t,f}$ are the number of existing production and storage facilities, and transportation units respectively at grid point g.

4.1.7 Non-anticipativity constraints

The multi-stage stochastic programming model includes five time periods and 81 scenarios. Each time period is mapped to each stage. It is assumed that the demand is known at the first-stage, while at the next stages different corrective actions are taken according to unique demand values of all scenarios. The decision variables associated with this discrete scenario will be similar up to the first time period. The following constraints guarantee this condition:

$$V_{q,ts1,sc} = V_{q,ts1,sc+1}, \forall o,ts,sc : 1 < sc < 81 \tag{24}$$

where V is any decision variable presented in the model. The index q denotes other indices incorporated in a particular variable such as e, g, g', g'', p, s, t, and h.

The demand uncertainty encountered in the second time period yields three different sets of scenarios:

$$\begin{aligned} V_{q,ts2,sc} &= V_{q,ts2,sc+1}, \forall o,ts,sc : 1 < sc < 27 \\ V_{q,ts2,sc} &= V_{q,ts2,sc+1}, \forall o,ts,sc : 27 < sc < 54 \\ V_{q,ts2,sc} &= V_{q,ts2,sc+1}, \forall o,ts,sc : 54 < sc < 81 \end{aligned} \tag{25}$$

In the next time periods the demand uncertainty is forming 3^{ts-1} different sets of scenarios. The following constraints guarantee this condition:

$$\begin{aligned} V_{q,ts,sc} &= V_{q,ts,sc+1}, \forall o,ts,sc : i < sc < k \cdot i, i = 1 \cdots \vdots \\ V_{q,ts,sc} &= V_{q,ts,sc+1}, \forall o,ts,sc : k \cdot (i-1) < sc < k \cdot i, i = 2, \ldots 3^{ts-1} \\ k &= {}^{81}/_{3^{ts-1}} \end{aligned} \tag{26}$$

In the last time period, there will be a unique set of variables for each of the 81 scenarios. These sets of variables will yield 81 different hydrogen network configurations.

4.2 Objective function

The expected total network costs of the HSC (TotalCost) of the HSC network is given as follows:

$$\text{Total Cost} = \min\{(\text{PC} + \text{SC} + \text{TC} + \text{ESC} + \text{EMC} + \text{PenC})/\text{NP}\} \tag{27}$$

The right-hand side of Eq. (27) contains the costs of hydrogen production (PC), transport (TC), storage (SC), energy sources (ESC), emission fees (EMC), and a penalty cost (PenC), divided by number of time periods (NP). The objective is to minimize the total costs by finding the combination of network components that satisfies the local hydrogen demand while satisfying the constraints.

Each production plant has an associated capital and operating cost. The total daily production cost is given by:

$$\text{PC} = \sum_{ts,g,p,h,f}\left(\frac{1}{\text{LR}}\left(\text{PCC}_{p,h,f}\cdot\text{InPF}_{ts,g,p,h,f}\cdot\text{AF}_p\right)\Big/\text{OP} + \sum_{sc}\rho_{sc}\cdot\text{HP}_{sc,ts,g,p,h,f}\cdot\text{POC}_{p,h,f}\right) \tag{28}$$

where $\text{PCC}_{p,h,f}$ represents the capital cost of facility p size h, producing hydrogen in form f, LR is the learning rate that takes into account the cost reduction of facilities while the experience accumulates with time. AF_p is an annuity factor for facility p, OP represents the operating period, and $\text{POC}_{p,h,f}$ denotes the hydrogen production cost in form f at facility p size h, ρ_{sc} is scenario probability.

The total hydrogen storage cost is calculated as:

$$\text{SC} = \sum_{ts,g,s,f}\left(\frac{1}{\text{LR}}\left(\text{SCC}_{s,f}\cdot\text{InSF}_{ts,g,s,f}\cdot\text{AF}_s\right)\Big/\text{OP} + \sum_{sc}\rho_{sc}\cdot\text{HSInv}_{sc,ts,g,s,f}\cdot\text{OC}_{s,f}\right)\frac{-b\pm\sqrt{b^2-4ac}}{2a} \tag{29}$$

where $\text{SCC}_{s,f}$ denotes the capital cost for storage facility s holding hydrogen in the form f, AF_s is annuity factor for the s storage facility, $\text{SOC}_{s,f}$ is the operating cost to store 1 kg of hydrogen in the form f at storage facility s.

The total distribution cost, calculated as the sum of the operating and capital costs, is given by:

$$\text{TC} = \sum_{ts,g,t,f}\left(\left(\text{TCC}_{t,f}\cdot\text{InTU}_{ts,g,t,f}\cdot\text{AF}_t\right)/\text{OP}\right) + \text{FC} + \text{LC} + \text{MC} \tag{30}$$

where $\text{TCC}_{t,f}$ denotes the capital cost of transport mode t for the distribution of hydrogen in form f, AF_t is an annuity factor for transport mode t, FC is the fuel cost, LC is labour cost, MC is maintenance cost.

The daily fuel cost for all scenarios and time periods is calculated as follows:

$$\text{FC} = \sum_{sc,ts,g,g',t,f}\rho_{sc}\cdot\frac{\text{FP}_t}{\text{FET}_t}\cdot 2\text{Dis}_{g,g',t}\cdot\text{HF}_{sc,ts,g,g',t,f}\Big/\text{TCap}_{t,f} \tag{31}$$

where FP_t represents fuel price for transportation mode t, FET_t denotes the fuel economy for transportation mode t.

The labor cost for all scenarios and time periods is calculated as:

$$LC = \sum_{sc,ts,g,g',t,f} \rho_{sc} \cdot DW_t \cdot HF_{sc,ts,g,g',t,f} \left(\frac{2Dis_{g,g',t}}{AvS_t} + LUT_t \right) \Big/ TCap_{t,f} \tag{32}$$

where DW_t represents the driver wage for transportation mode t.

The maintenance cost for all scenarios and time periods is calculated as:

$$MC = \sum_{sc,ts,g,g',t,f} \rho_{sc} \cdot ME_t \cdot 2Dis_{g,g',t} \cdot HF_{sc,ts,g,g',t,f} \Big/ TCap_{t,f} \tag{33}$$

where ME_t denotes maintenance cost for transportation mode t.

The price for the energy source consumed for all scenarios and time periods is calculated by:

$$\begin{aligned} ESC = & \sum_{sc,ts,g'',g,p,e} PESAv_{sc,ts,g'',g,p,e} \left(ESDis_e \cdot Dis_{g'',g} + ESCost_e \right) \\ & + \sum_{sc,ts,g'',g,p,e} PESIm_{sc,ts,g,p,e} \cdot ESICost_e \end{aligned} \tag{34}$$

where $ESICost_e$ represents the energy source e import price, $ESCost_e$ denotes the energy source e price, generated locally, $ESDis_e$ is the delivery price for energy source e, and $Dis_{g'',g}$ is the distance between grid points.

Based on the work of De-León Almaraz et al. [15], the total daily greenhouse gas (GHG) emission is associated with the GHG emitted during production, storage and transportation of HSC network at period ts:

$$TotalCO_{2sc,ts} = PCO_{2sc,ts} + SCO_{2sc,ts} + TCO_{2sc,ts}, \forall sc, ts \tag{35}$$

where $TotalCO_{2sc,ts}$ is the total daily amount of emitted GHG in the HSC network during time period ts and scenario sc, $PCO_{2sc,ts}$ is the daily GHG emission from the production sites during time period ts and scenario sc, $SCO_{2sc,ts}$ is the daily GHG emission from the storage sites during time period ts and scenario sc, $TCO_{2sc,ts}$ is the daily GHG emission from distribution of hydrogen during time period ts and scenario sc.

The GHG emissions in production sites are associated with the produced hydrogen of the form f by the each production facility p size h at grid point g during time period ts and scenario sc, and the total daily GHG emissions in production sites:

$$PCO_{2sc,ts} = \sum_{g,p,h,f} HP_{sc,ts,g,p,h,f} \cdot GEP_{p,f}, \forall sc, ts \tag{36}$$

where $GEP_{p,f}$ is the amount of GHG emitted per kg H_2 produced in the form f in production facility p.

The total daily GHG emissions to store produced hydrogen is calculated as:

$$\mathrm{SCO}_{2sc,ts} = \sum_{g,p,h,f} \mathrm{HP}_{sc,ts,g,p,h,f} \cdot \mathrm{GES}_f, \forall sc, ts \tag{37}$$

where GES_f is the amount of GHG emitted to store 1 kg H_2 in the form *f*.

The total daily transport GHG emissions are determined from:

$$\mathrm{TCO}_{2sc,ts} = \sum_{g,g',t,f} \rho_{sc} \cdot \mathrm{GET}_t \cdot 2\mathrm{Dis}_{g,g',t} \cdot \mathrm{HF}_{sc,ts,g,g',t,f} \big/ \mathrm{TCap}_{t,f} \tag{38}$$

where GET_t is the amount of GHG emitted per km traveled distance of transportation mode *t*.

The final emissions fee from the HSC for all scenarios and time periods is calculated as:

$$\mathrm{EMC} = \sum_{sc,ts} \rho_{sc} \cdot \mathrm{TotalCO}_{2sc,ts} \cdot \mathrm{Tax}_{ts} \tag{39}$$

where Tax_{ts} represents the tax for the CO_2 emissions for time period *ts*. It is assumed that Tax_{ts} is changing in time according to:

$$\mathrm{Tax}_{ts} = \mathrm{CurTax}\,(1 + \mathrm{InRate}\,(ts - 1)), \forall ts \tag{40}$$

where CurTax represents current value of emissions fee for 1 kg CO_2, InRate represents the increasing rate.

To analyze the economic value of supply security, a penalty method is applied. The penalty is calculated as follows:

$$\mathrm{PenC} = \mathrm{Pen} \cdot \sum_{sc,ts,g,f} \rho_{sc} \cdot \mathrm{HI}_{sc,ts,g,f} \tag{41}$$

where Pen is calculated as,

$$\mathrm{Pen} = \sum_{sc,ts,g} \frac{\gamma_{ts} \cdot \mathrm{PN}_{sc,ts,g} \cdot \mathrm{TT} \cdot \mathrm{NetIn}}{\mathrm{AvH} \cdot \mathrm{HD}_{sc,ts,g}} \tag{42}$$

where AvH represents the average number of members in one household (family), TT is determined as the time used by a passenger transport by members of one household. NetIn is the average income per household. All relevant data can be found in Appendix A and B.

5 Results and discussion

To examine the HSC configurations, the model is setup as an MILP consisting of 5,539,256 constraints, 3,490,596 continuous variables, 880,320 binary variables. AIMMS is used as optimization platform and CPLEX 12.8 is selected as the solver. The result section consists two parts. First, the optimal hydrogen infrastructure for both configurations is discussed in more detail. Second, the effect of the demand uncertainty is analyzed and discussed.

5.1 The optimal HSC configuration

The scenario-based approach given by Eqs. (2)–(42) is used to model the demand uncertainty. This approach represents a collection of outcomes for all stochastic events taking place in the model with its associated probability, organized into a scenario tree. For each HSC configurations, three demand scenarios referred to as "high" (+20% expected demand), "medium" (expected demand), "low" (–20% expected demand) scenarios over five time periods of planning horizon are presented.

As mentioned before, the hydrogen demand is assumed to be known during the first time period (2020–2026). This demand is calculated by 6.7% penetration of FCEVs into passenger transport. Hydrogen demand is met by large-scale SMR-based plants located in Stuttgart, Munich, Berlin, Rostock, Mainz, Dresden and two large-scale SMR plants in Cologne (eight plants total). During the second time period, only three demand scenarios are examined: 14.0, 11.6 and 9.3% penetration (2026–2032). The demand level is met by additional large-scale SMR plants in Stuttgart, Rostock, Mainz and by two large-scale SMR in Munich and Cologne (seven plants total). Nine scenarios are examined for the third time period (2032–2038), the demand level is presented as 19.9, 16.6 and 13.3% penetration. Only three large-scale SMR plants are installed (Frankfurt, Kiel, Erfurt). For the rest of the time, additional plants do not need to be installed. The optimal number of production plants by 2050 is 18 large-scale SMR plants to fulfill the required demand. Hydrogen storage for 10 days requires 166 super-insulated spherical tanks installed at the first time period. Additionally, 227 transportation units are required to transport the liquid hydrogen from production- to storage sites which are added in different time periods (see Table B.6). The expected total cost for the multi-stage stochastic optimization model equals 27.25 M$ per time period. The overall price of hydrogen varies from 5.11$ to 7.42$ per kg.

The second configuration of the model includes the WE-based technology, whose current level of technological development only allows small-scale production capacities. The total number of WE-based plant equals 857 units, which are installed at the first time period at each grid points. Moreover, 214 transportation units are required to transport the liquid hydrogen to satisfy hydrogen demand. Note that hydrogen demand is satisfied by local production. The expected total cost equals 52.97 M$ per time period. However, it is further assumed that the electricity consumption to produce 1 kg of hydrogen can vary from 47.3 to 44.3 kWh depending on the scale of plant, and all production size scales is allowed [33]. The network requires 18 large-scale electrolysis-based plants to produce liquid hydrogen to satisfy demand by 2050. During the first time period, hydrogen demand is satisfied by five large-scale WE plants (Stuttgart, Munich, Rostock, Cologne, Dresden) and two large-scale WE-based plants located in Mainz. Additional eight large-scale WE plants (Stuttgart, Berlin, Potsdam, Rostock, Hannover, Cologne, Kiel, Erfurt) and two large-scale WE plants in Munich are installed at the second time period, and one large-scale WE located in Hannover is installed at

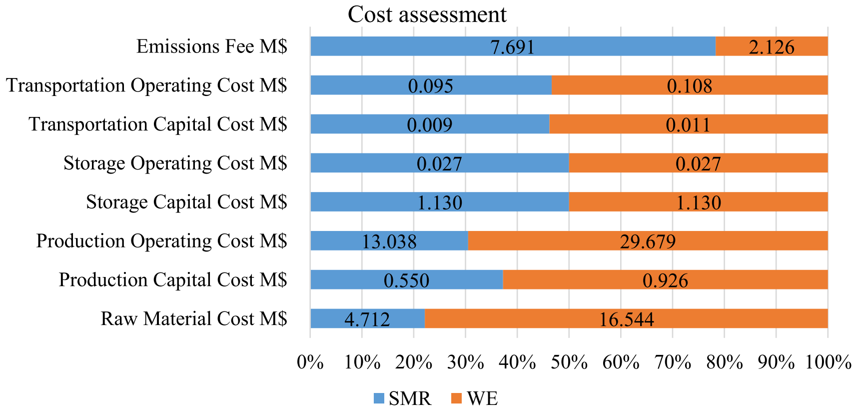

Figure 7: Cost assessment of HSC: SMR versus WE technologies.

the third time period. Moreover, the model requires 166 super-insulated spherical tanks and 270 transportation units. The expected total cost for multi-stage stochastic optimization is 50.55 M$ per time period (see Table B.7). The hydrogen cost lies between 9.49$ and 13.77$ per kg. Figure 7 shows of the cost assessment for both configurations. A small emissions fee for WE-based hydrogen production is observed, while the price of production sites and raw material is two times higher than for SMR-based technologies.

5.2 Effects of demand uncertainty

The concepts of EVPI and VSS are applied to evaluate the stochastic optimization results and compare them to their deterministic counterpart (see Section 3.1). Mathematically, the EVPI is defined as the difference between the wait-and-see (WS) solution and recourse problem (RP), and the VSS is the value obtained by taking the difference between the result of using an expected value solution (EEV) and the RP. The WS solution represents the expected value of the deterministic solution that can be determined after simulation of each scenario individually. EEV is obtained by calculating the expected value of the deterministic solution while replacing all random variables at the first-stage by their expected values and allowing a second-stage decision to be chosen optimally. In addition, the RP solution is the result of the stochastic optimization. For the penalty cost that is lower than the calculated value of *PenC*, the results of the WS, RP and EEV are small because the import of hydrogen would satisfy a demand with lower costs than if hydrogen would be produced locally. However, taking into consideration the expected penalty cost, EVPIs for both configurations are more pronounced, adding up 4.2 and 6.7 M$ respectively, which are corresponding to 15–25% of the infrastructure investments. A high EVPI represents the importance of accurate projections to minimize infrastructure investments in the long run. Moreover,

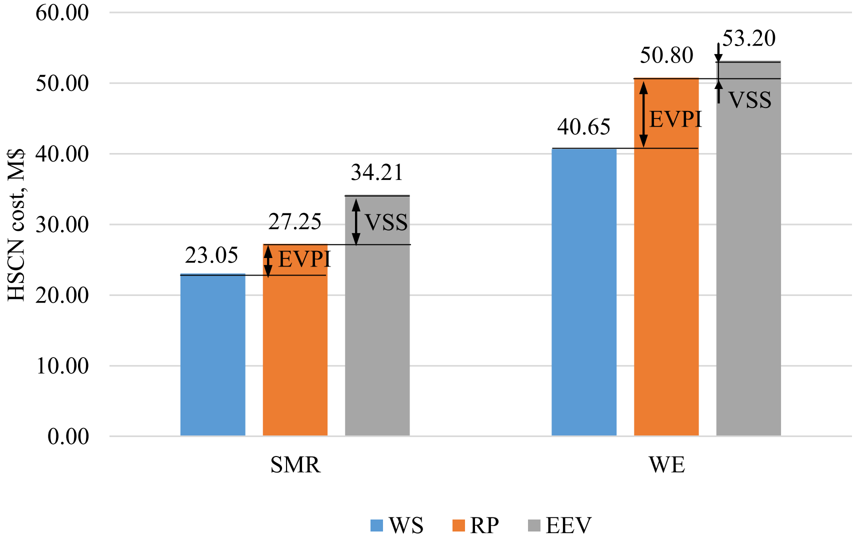

Figure 8: WS, RP and EEV solutions for the evaluated network configurations.

the VSS shows benefits of a stochastic approach for the model presented in this work, compared to a deterministic approach, up 7 M$ of infrastructure investments savings, corresponding 26% of total investments. Due to the high costs of the second configuration, part of the hydrogen demand is fulfilled by imports, which is the cause of its lower VSS. EVPI and VSS results are presented in Figure 8.

6 Conclusions

In this work, a multi-stage stochastic MILP is presented to assist the strategic decision-making for the design of a hydrogen infrastructure for the transportation sector in Germany. Based on univariate sensitivity analysis applied in the deterministic model [22], hydrogen demand is considered as the uncertain parameter in the stochastic formulation, and its effect on the infrastructure investments is analyzed up to 2050. A scenario-based approach is applied to capture demand uncertainty over this extended period of time. Five time periods and 81 scenarios are considered for the demand. Each time period is represented as six-year interval starting from 2020 until 2050. It was assumed that the demand is known at the first-stage, when at the next stages different corrective actions can be taken according to unique demand values of all scenarios. The value of the stochastic solution for each configuration shows significant benefits, where 26% of infrastructure investments savings can be made when incorporating demand uncertainty. Two HSC configurations are considered, which are analyzed and compared to each other according to production types. As the results show, a small emissions fee for water electrolysis is observed, while the price of production sites and raw material is two times higher than for steam methane reforming based technologies. However, the use of limited fossil fuels and large CO_2 emissions will shift the optimal network configuration from SMR to water electrolysis based technology according to its progress rate.

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