Design of Hydrogen Supply Chains under Demand Uncertainty – A Case Study of Passenger Transport in Germany

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Abstract

A strategy for the design of a hydrogen supply chain (HSC) network in Germany incorporating the uncertainty in the hydrogen demand is proposed. 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 vs 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: Hydrogen supply chain design, Mixed Integer Linear Programming, Stochastic optimization, Fuel infrastructures, Water electrolysis technology.

1. Introduction

The population is constantly growing and consuming more energy year after year (Pregger et al., 2013; Schill, 2014). 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. 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 (Lahnaoui et al., 2018). 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 (Grüger et al., 2018; Wulf et al., 2018). 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 (Emonts et al., 2019; Reuß et al., 2019; Robinius et al., 2018). 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 (International Energy Agency, 2015). It stands behind the development of a hydrogen supply chain (HSC) considering safety, economic and environmental impact issues (Ball et al., 2007).

Many studies in the area of HSC design focus on network evaluation using steady-state simulation (Lahnaoui et al., 2018; Robles et al., 2016; Wulf and Kaltschmitt, 2018). The work of Hugo et al. considers all possible hydrogen alternatives for an optimal hydrogen infrastructure design (Hugo et al., 2005). 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 (Kim and Moon, 2008). 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 (De-León Almaraz et al., 2013). 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 (Almansoori and Betancourt-Torcat, 2016; Almansoori and Shah, 2009). 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 (Lahnaoui et al., 2018; Reuß et al., 2019).

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 (Grossmann, 2005; You and Grossmann, 2013). 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 (Kim et al., 2008). 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 (Almansoori and Shah, 2012).

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 (Ochoa Bique and Zondervan, 2018). Moreover, the best trade-off solution of multi-objective optimizations shows significant dominance of water electrolysis technology against the rest (Bique et al., 2018). This work is an extension of a previous model 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 (Sahinidis, 2004). 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 (Maire, 2013):

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

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

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 (Almansoori and Shah, 2012; Dayhim et al., 2014; Kim and Moon, 2008). 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. Fig. 1 shows the sensitivities of all selected parameters on the objective function, while Fig. 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.

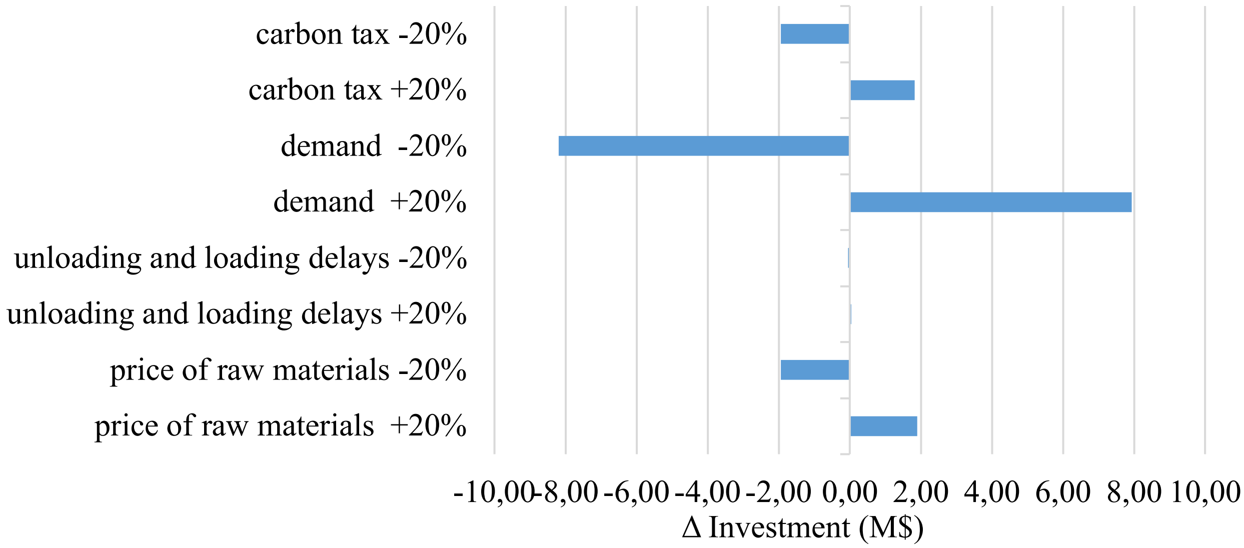

Fig. 1. Sensitivities of selected parameters on objective function (total daily cost)

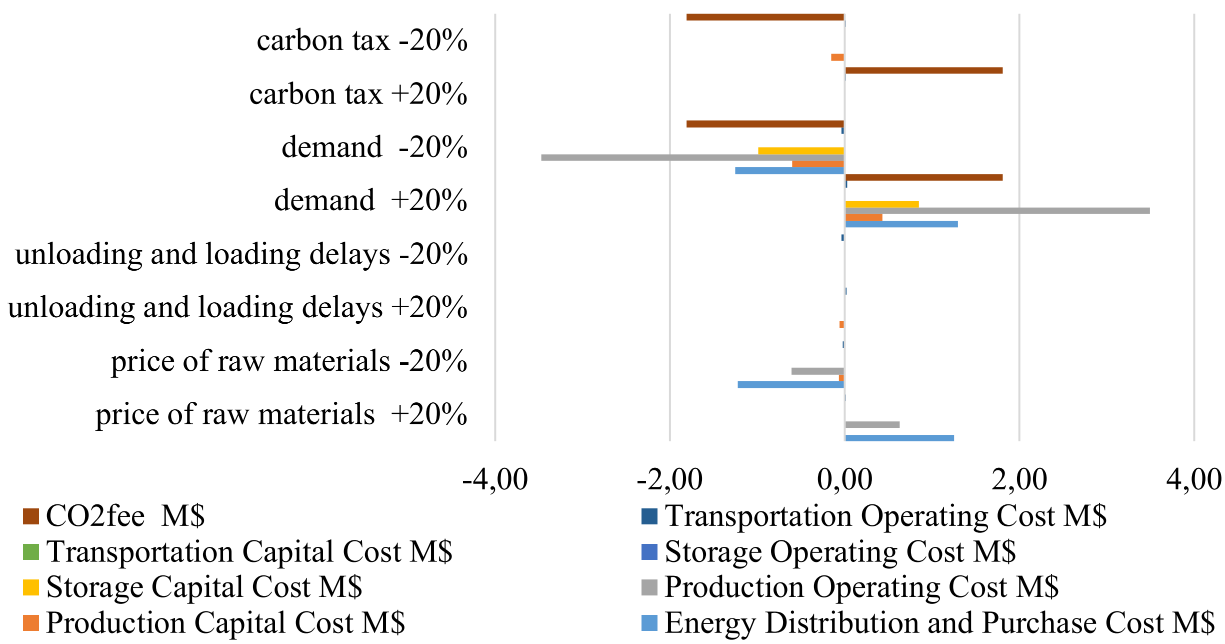

Fig. 2. Sensitivities of selected parameters on other decision variables in the model

3. Network description and problem statement

The analysis of previous studies (Bique et al., 2018; Ochoa Bique and Zondervan, 2018) 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 vs 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 Fig. 3).

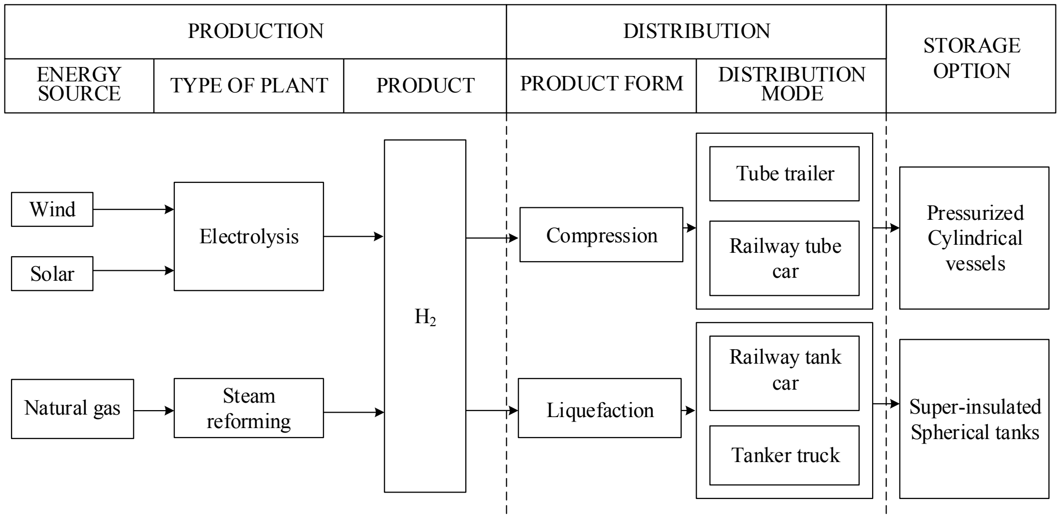

Fig. 3. Structure of the hydrogen supply and delivery chain

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 eighty-one scenarios. Each time period represents a 6-year interval starting from 2020 until 2050 (see Fig. 4).

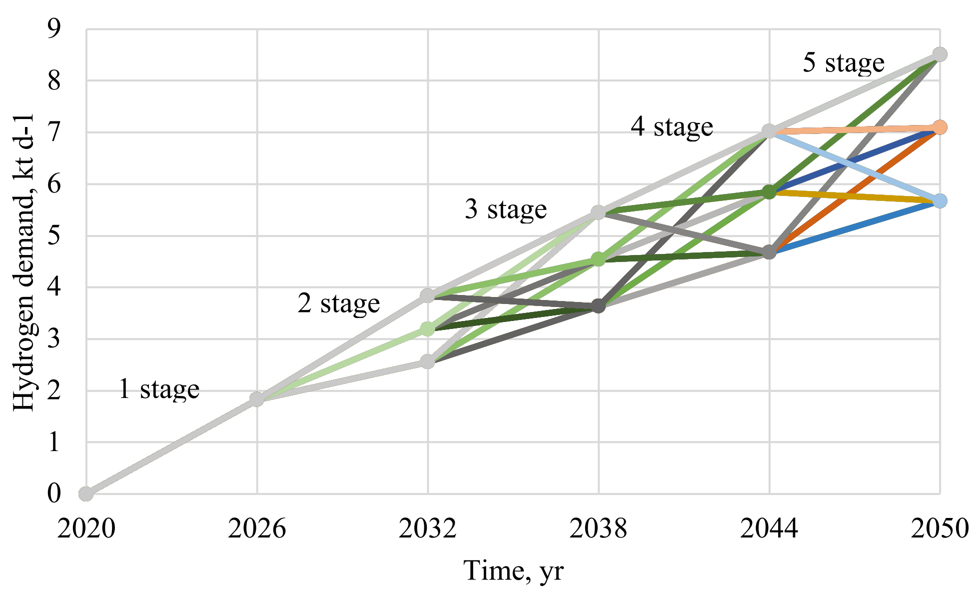

Fig. 4. Demand scenario tree (trajectory)

Each scenario has a uniquely defined demand value as shown Fig. 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 (Grossmann et al., 2017) 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 (Smith and Coit, 2010). 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 (Birge and Louveaux, 2011).

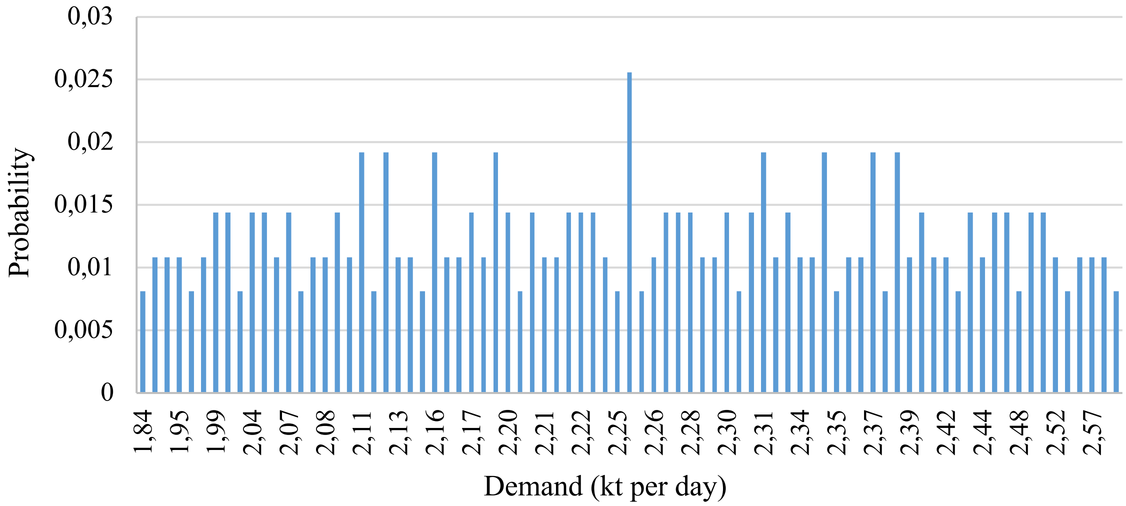

Fig. 5. Demand distribution. Values shown correspond to total demand for each scenario up to 2050

The data was collected from the Federal Statistical Office of Germany (Statistisches Bundesamt, n.d.), the Fraunhofer Institute for Solar Energy Systems ISE (ISE, n.d.), Almansoori and Betancourt-Torcat (Almansoori and Betancourt-Torcat, 2016), Ruth (Ruth et al., 2009).

3.2. Formulation of the HSC

In Fig. 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 (Bique et al., 2018).

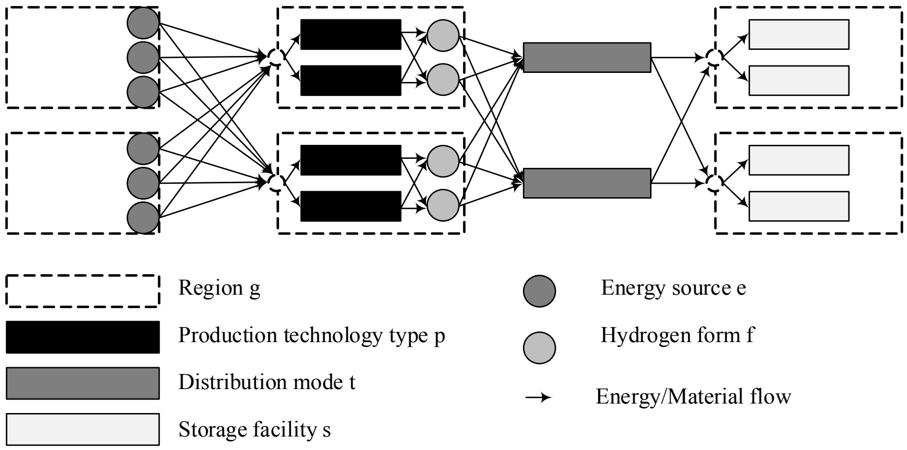

Fig. 6. Model superstructure

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:

$$\begin{aligned} &\min c^1 x^1 + E_{\Omega}\left[c^2 x^2 + \ldots + c^H x^H \right] \\ &\text{s.t.} \qquad W^1 x^1 = h^1, \\ &T^{t-1} x^{t-1} + W^t x^t = h^t, \quad t = 2, \ldots, H, \\ &x^1 \geq 0, x^t \geq 0, \quad t = 2, \ldots, H; \end{aligned} \tag{1}$$

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:

$$ESD_{sc,ts,g,p,e} = \sum_{f,h} HP_{sc,ts,g,p,h,f}\, \alpha_{e,p,h}, \qquad \forall e, p, g, ts, sc \tag{2}$$

where $HP_{sc,ts,g,p,h,f}$ 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.

$$ESD_{sc,ts,g,p,e} \leq \sum_{g''} PESAv_{sc,ts,g'',g,p,e} + PESIm_{sc,ts,g,p,e}, \quad \forall e,p,g,ts,sc \tag{3}$$

In (3) $PESAv_{sc,ts,g'',g,p,e}$ 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*, $PESIm_{sc,ts,g,p,e}$ 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:

$$\sum_{g} PESAv_{sc,ts,g'',g,p,e} \leq ESAv_{ts,g'',e}, \quad \forall e,p,g'',ts,sc \tag{4}$$

where $ESAv_{ts,g'',e}$ 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. (Lahnaoui et al., 2018). The hydrogen demand by grid point can be calculated as follows:

$$HD_{sc,ts,g} = \gamma_{ts} PN_{sc,ts,g} AvD_{ts} \cdot FE, \quad \forall g,ts,sc \tag{5}$$

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:

$$HD_{sc,ts,g} \leq \sum_{f} \left(HD_{sc,ts,g,f} + HI_{sc,ts,g,f} \right), \forall g,ts,sc \tag{6}$$

$HD_{sc,ts,g,f}$ 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*, $HI_{sc,ts,g,f}$ 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:

$$HD_{sc,ts,g,f} \leq \sum_{t,g'} HF_{sc,ts,g',g,t,f}, \quad \forall f,g,ts,sc \tag{7}$$

where $HF_{sc,ts,g',g,t,f}$ 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:

$$HP_{sc,ts,g,f} = \sum_{p,h} HP_{sc,ts,g,p,h,f}, \qquad \forall g,f,ts,sc \tag{8}$$

where $HP_{sc,ts,g,f}$ represents the hydrogen generation in form *f* at grid point *g* during time period *ts* for scenario *sc*, $HP_{sc,ts,g,p,h,f}$ 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:

$$MinPCap_{p,h} NPF_{ts,g,p,h,f} \le HP_{sc,ts,g,p,h,f} \le MaxPCap_{p,h} NPF_{ts,g,p,h,f}, \quad \forall g,p,f,ts,sc \tag{9}$$

where $MinPCap_{p,h}$, $MaxPCap_{p,h}$ is the min/max production capacity for hydrogen production facility *p* size *h*, $NPF_{ts,g,p,f}$ 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:

$$MinHF_{t,f} X_{sc,ts,g,g',t,f} \le HF_{sc,ts,g,g',t,f} \le MaxHF_{t,f} X_{sc,ts,g,g',t,f}, \quad \forall sc,ts,g,g',t,f \tag{10}$$

where $MinHF_{t,f}$, $MaxHF_{t,f}$ 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:

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

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

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

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:

$$HP_{sc,ts,g,f} \ge \sum_{t,g'} HF_{sc,ts,g,g',t,f}, \qquad \forall g,f,ts,sc \tag{14}$$

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:

$$NTU_{ts,g,g',t,f} \geq \frac{HF_{sc,ts,g,g',t,f}\left(\frac{2Dis_{g,g',t}}{AvS_t} + LUT_t\right)}{MA_t \cdot TCap_{t,f}} + ExT_{sc,ts,g,g',t,f}, \quad \forall sc,ts,g,g',t,f \tag{15}$$

where $Dis_{g,g',t}$ 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, $TCap_{t,f}$ is capacity of transportation unit t to distribute produced hydrogen in form f, $ExT_{sc,ts,g,g',t,f}$ is continuous variable in scenario sc with value between 0 and 1, which is used to take an integer value for $NTU_{ts,g,g',t,f}$ (modification was suggested by De-León Almaraz et al., 2013).

4.1.5. Hydrogen storage constraints

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

$$MinSCap_{s,f} NSF_{ts,g,s,f} \leq HSInv_{sc,ts,g,s,f} \leq MaxSCap_{s,f} NSF_{ts,g,s,f} \quad \forall g,s,f,ts,sc \tag{16}$$

where $NSF_{ts,g,s,f}$ denotes the number of storage facilities s holding hydrogen in form f at grid point g during time period ts, and $MinSCap_{s,f}$, $MaxSCap_{s,f}$ represent the minimum and maximum capacities of storage facility s for holding hydrogen in the from f, $HSInv_{sc,ts,g,s,f}$ 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,

$$\sum_s HSInv_{sc,ts,g,s,f} \geq \tau \cdot HD_{sc,ts,g,f}, \quad \forall f,g,ts,sc \tag{17}$$

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:

$$NPF_{ts,g,p,h,f} = NPF_{(ts-1),g,p,h,f} + InPF_{ts,g,p,h,f}, \quad \forall ts,g,p,h,f : ts \neq ts1 \tag{18}$$

$$NSF_{ts,g,s,f} = NSF_{(ts-1),g,s,f} + InSF_{ts,g,s,f}, \quad \forall ts,g,s,f : ts \neq ts1 \tag{19}$$

$$InTU_{ts,g,t,f} = \sum_{g'} NTU_{ts,g,g',t,f} - \sum_{g'} NTU_{(ts-1),g,g',t,f}, \quad \forall ts,g,t,f : ts \neq ts1 \tag{20}$$

where $InPF_{ts,g,p,h,f}$, $InSF_{ts,g,s,f}$ and $InTU_{ts,g,t,f}$ 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,

$$NPF_{ts1,g,p,h,f} = ExNPF_{g,p,h,f} + InPF_{ts1,g,p,h,f}, \quad \forall g,p,h,f \tag{21}$$

$$NSF_{ts1,g,s,f} = ExNSF_{g,s,f} + InSF_{ts1,g,s,f}, \quad \forall g,s,f \tag{22}$$

$$InTU_{ts1,g,t,f} = \sum_{g'} NTU_{ts1,g,g',t,f} - ExTU_{g,t,f}, \quad \forall g,t,f \tag{23}$$

where $ExNPF_{g,p,h,f}$, $ExNSF_{g,s,f}$ and $ExTU_{g,t,f}$ 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 eighty-one 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:

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

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:

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

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

$$V_{q,ts,sc} = V_{q,ts,sc+1}, \quad \forall o, ts, sc : i < sc < k \cdot i, \ i = 1$$

$$\ldots \vdots \tag{26}$$

$$V_{q,ts,sc} = V_{q,ts,sc+1}, \quad \forall o, ts, sc : k \cdot (i-1) < sc < k \cdot i, \quad i = 2, \ldots 3^{ts-1}$$

$$k = 81/3^{ts-1}$$

In the last time period, there will be a unique set of variables for each of the eighty one scenarios. These sets of variables will yield eighty one 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:

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

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:

$$PC = \sum_{ts,g,p,h,f} \left(\frac{1}{LR} \left(PCC_{p,h,f} InPF_{ts,g,p,h,f} AF_p \right) / OP + \sum_{sc} \rho_{sc} HP_{sc,ts,g,p,h,f} POC_{p,h,f} \right) \tag{28}$$

where $PCC_{p,h,f}$ 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 $POC_{p,h,f}$ 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:

$$SC = \sum_{ts,g,s,f} \left(\frac{1}{LR} \left(SCC_{s,f} InSF_{ts,g,s,f} AF_s \right) / OP + \sum_{sc} \rho_{sc} HSInv_{sc,ts,g,s,f} SOC_{s,f} \right) \tag{29}$$

where $SCC_{s,f}$ denotes the capital cost for storage facility *s* holding hydrogen in the form *f*, AF_s is annuity factor for the *s* storage facility, $SOC_{s,f}$ 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:

$$TC = \sum_{ts,g,t,f} \left(\left(TCC_{t,f} InTU_{ts,g,t,f} AF_t \right) / OP \right) + FC + LC + MC \tag{30}$$

where $TCC_{t,f}$ 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:

$$FC = \sum_{sc,ts,g,g',t,f} \rho_{sc} \frac{FP_t}{FET_t} 2Dis_{g,g',t} HF_{sc,ts,g,g',t,f} \Big/ TCap_{t,f} \tag{31}$$

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:

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

where DW_t represents the driver wage for transportation mode t.

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

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

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,

$$ESC = \sum_{sc,ts,g'',g,p,e} PESAv_{sc,ts,g'',g,p,e} (ESDis_e \, Dis_{g'',g} + ESCost_e) + \sum_{sc,ts,g'',g,p,e} PESIm_{sc,ts,g,p,e} ESICost_e \tag{34}$$

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. (De-León Almaraz et al., 2013), the total daily greenhouse gas (GHG) emission is associated with the GHG emitted during production, storage and transportation of HSC network at period ts:

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

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:

$$PCO2_{sc,ts} = \sum_{g,p,h,f} HP_{sc,ts,g,p,h,f} GEP_{p,f} \quad , \forall sc, ts \tag{36}$$

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:

$$SCO2_{sc,ts} = \sum_{g,p,h,f} HP_{sc,ts,g,p,h,f} GES_f \quad , \forall sc, ts \tag{37}$$

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:

$$TCO2_{sc,ts} = \sum_{g,g',t,f} \rho_{sc} \cdot GET_t 2Dis_{g,g',t} HF_{sc,ts,g,g',t,f} / TCap_{t,f} \tag{38}$$

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:

$$EMC = \sum_{sc,ts} \rho_{sc} TotalCO2_{sc,ts} Tax_{ts} \tag{39}$$

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:

$$Tax_{ts} = CurTax(1 + InRate(ts - 1)) \quad , \forall ts \tag{40}$$

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:

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

where Pen is calculated as,

$$Pen = \sum_{sc,ts,g} \frac{\gamma_{ts} PN_{sc,ts,g} \cdot TT \cdot NetIn}{AvH \cdot HD_{sc,ts,g}} \tag{42}$$

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 the Appendix A, 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 discuss 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 eq. (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 2 large-scale SMR plants in Cologne (8 plants total). During the second time period, only three demand scenarios are examined: 14.0, 11.6 and 9.3 percent penetration (2026-2032). The demand level is met by additional large-scale SMR plants in Stuttgart, Rostock, Mainz and by 2 large-scale SMR in Munich and Cologne (7 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 percent penetration. Only 3 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 kWh to 44.3 kWh depending on the scale of plant, and all production size scales is allowed (Saba et al., 2018). 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 5 large-scale WE plants (Stuttgart, Munich, Rostock, Cologne, Dresden) and 2 large-scale WE-based plants located in Mainz.

Additional 8 large-scale WE plants (Stuttgart, Berlin, Potsdam, Rostock, Hannover, Cologne, Kiel, Erfurt) and 2 large-scale WE plants in Munich are installed at the second time period, and 1 large-scale WE located in Hannover is installed at 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$ to 13.77$ per kg. Fig. 7 shows of the cost assessment for both configurations. A high price of production sites and raw material of WE-based hydrogen production vs SMR-based, considering small emissions fee can be observed.

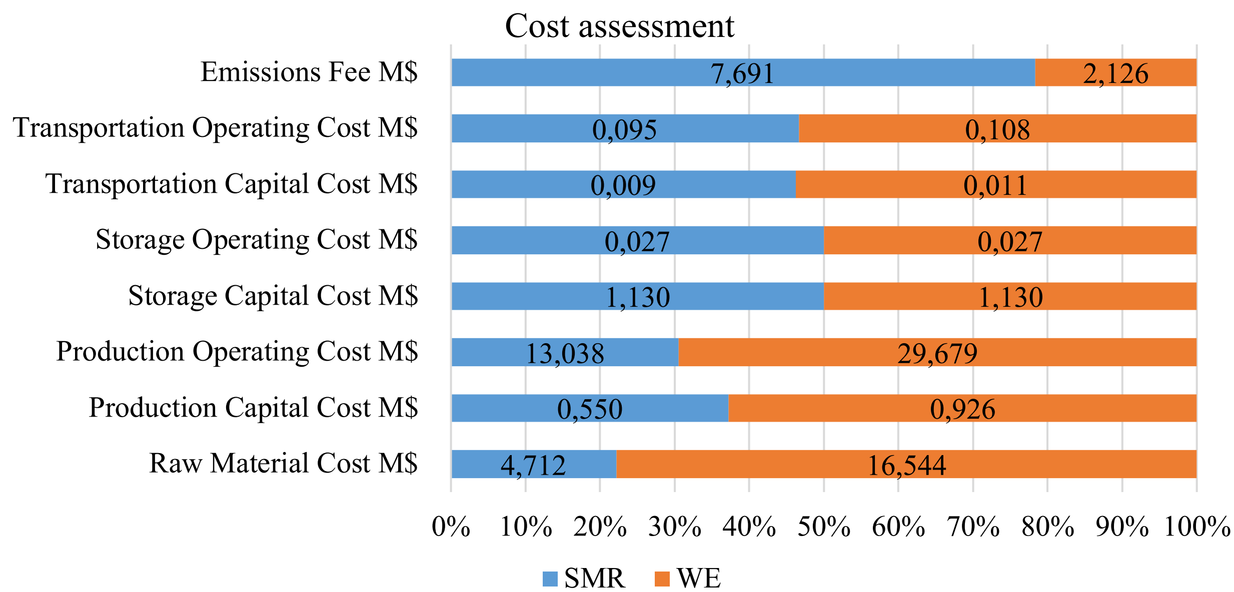

Fig. 7. Cost assessment of HSC: SMR vs WE technologies

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, 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 Fig. 8.

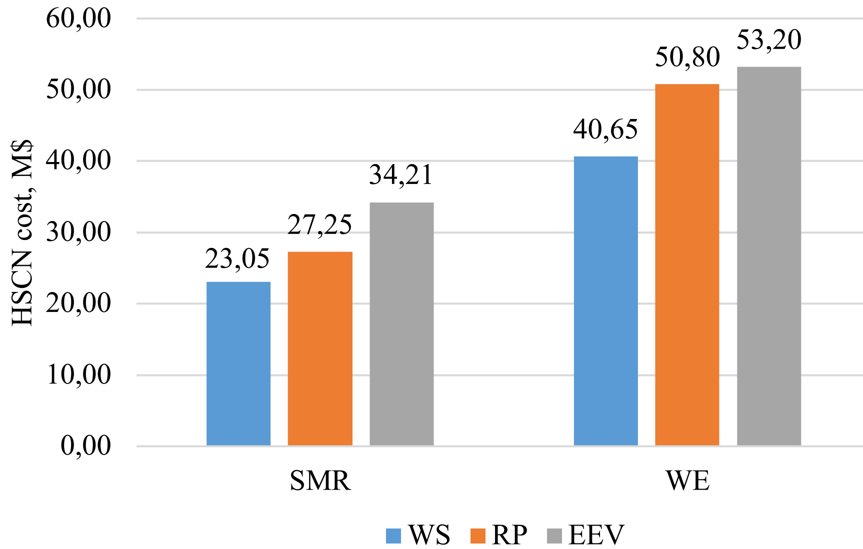

Fig. 8. WS, RP and EEV solutions for the evaluated network configurations

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 a sensitivity analysis, 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 eighty-one scenarios are considered for the demand. Each time period is represented as 6-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 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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Appendix A.
Nomenclature

Indices	
e	type of energy source
f	type of hydrogen physical form
g	grid points, each grid point represents German state
p	type of hydrogen production facility
h	size factor
s	type of storage facility
t	type of transportation mode
sc	demand scenarios
ts	time periods of the planning horizon
Abbreviation	
BEV	battery electrical vehicles
BG	biomass gasification
CG	coal gasification
CO_2	carbon dioxide
EEV	expected result of using the expected value solution
EVPI	expected value of perfect information
FCEV	fuel cell electric vehicle
GHG	greenhouse gas
HSC	hydrogen supply chain
MILP	mixed integer linear programming
RP	recourse problem
SMR	steam methane reforming
VSS	value of the stochastic solution
WE	water electrolysis
WS	wait-and-see solution
Continuous variable	
ESC	total cost for the energy source consumed for hydrogen production [$ d^{-1}]
$ESD_{sc,ts,g,p,e}$	daily energy source e demand by grid point g for production technology p during time period ts for scenario sc [kWh d^{-1}]
EMC	final emissions fee [$ d^{-1}]
$ExT_{sc,ts,g,g',t,f}$	continuous variable in scenario sc with value between 0 and 1, which is used to take an integer value for $NTU_{ts,g,g',t,f}$
FC	daily fuel cost [$ d^{-1}]
$HD_{sc,ts,g,f}$	amount of hydrogen demand satisfied by network in the form f in grid point g at time period ts and scenario sc[kg d^{-1}]

$HF_{sc,ts,g,g',t,f}$	hydrogen flowrate in the form *f* from grid point *g* to *g'* via transportation mode *t* during time period *ts* for scenario *sc* [kg d^{-1}]
$HI_{sc,ts,g,f}$	amount of hydrogen imported from another country to satisfy hydrogen demand in form *f* in grid point *g* at time period *ts* and scenario *sc* [kg d^{-1}]
$HP_{sc,ts,g,f}$	hydrogen generation in the form *f* at grid point *g* during time period *ts* for scenario *sc* [kg d^{-1}]
$HP_{sc,ts,g,p,h,f}$	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* [kg d^{-1}]
$HSInv_{sc,ts,g,s,f}$	inventory of product *f* in the storage facility s at grid point *g* at time period *ts* and scenario *sc* [kg]
LC	labor cost [$ d^{-1}]
MC	maintenance cost [$ d^{-1}]
PC	daily production costs[$ d^{-1}]
$PCO_{2\,sc,ts}$	daily GHG emission from the production sites during time period *ts* and scenario *sc* [kg d^{-1}]
$PESAv_{sc,ts,g'',g,p,e}$	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* [unit e d^{-1}]
$PESIm_{sc,ts,g,p,e}$	flowrate importing energy source *e* to the grid point *g*, where production facility *p* is installed, during time period *ts* for scenario *sc* [unit e d^{-1}]
SC	the total hydrogen storage cost [$]
$SCO_{2\,sc,ts}$	daily GHG emissions from storage sites during time period *ts* and scenario *sc* [kg d^{-1}]
TC	daily distribution cost [$ d^{-1}]
$TCO_{2\,sc,ts}$	daily GHG emissions during hydrogen delivery at time period *ts* and scenario *sc* [kg d^{-1}]
TotalCost	total daily cost of HSC network [$ d^{-1}]
$TotalCO_{2\,sc,ts}$	total daily GHG emission of HSC network during time period *ts* and scenario *sc* [kg d^{-1}]

Integer variables

$InPF_{ts,g,p,h,f}$	number of new invested production facility *p* size *h* generating hydrogen in from *f* at grid point *g* during time period *ts*
$InSF_{ts,g,s,f}$	number of new invested storage facility *s* holding hydrogen in from *f* at grid point *g* during time period *ts*
$InTU_{ts,g,t,f}$	number of new invested transportation units *t* for hydrogen distribution in the form *f* at grid point *g* during time period *ts*
$NPF_{ts,g,p,h,f}$	total number of production facility *p* size *h* generating hydrogen in from *f* at grid point *g* during time period *ts*
$NSF_{ts,g,s,f}$	total number of storage facility *s* holding hydrogen in from *f* at grid point *g* during time period *ts*
$NTU_{ts,g,g',f,t}$	total number of transport mode *t* used for hydrogen distribution in the form *f* from *g* to *g'* during time period *ts*

Binary variables

$X_{sc,ts,g,g',t,f}$	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* in scenario *sc*, otherwise 0
$Q_{sc,ts,g,f}/W_{sc,ts,g,f}$	1 if product in form *f* is exported/imported during time period *ts* in scenario *sc*, otherwise 0

Parameters

AvD_{ts}	average distance travelled by personal car at time period *ts* [km y^{-1} $capita^{-1}$]
AvH	average number of members in one household

AvS_t	average speed of transportation mode t [km h^{-1}]
AF_p	annual factor for the facility p [%]
AF_s	annual factor for the s storage facility s [%]
AF_t	annual factor for the transport mode t [%]
$CurTax$	current value of emissions fee for 1 kg CO_2 [\$ kg^{-1}]
$Dis_{g'',g}$	distance between grid points [km]
$Dis_{g,g',t}$	distance between grid points depending of type of transport [km]
DW_t	driver wage, who drives transportation mode t [\$]
$ESAv_{ts,g'',e}$	the amount of available energy source e at grid point g at time period ts.
$ESCost_e$	energy source e price in year y, generated locally [\$ $unit^{-1}$ e]
$ESDis_e$	delivery price for energy source e [\$ $unit^{-1}$ km^{-1}]
$ESICost_e$	energy source e import price [\$ $unit^{-1}$]
FE	the fuel economy [kg H_2 km^{-1}]
FET_t	fuel economy for transportation mode t [unit km^{-1}]
FP_t	fuel price for transport mode t [\$ $unit^{-1}$]
$GEP_{p,f}$	GHG emitted in the production facility p to produce kg H2 in the form f [kg kg^{-1} H_2]
GES_f	GHG emitted in storage side to store kg H2 in the form f [kg kg^{-1} H_2]
GET_t	GHG emitted by transport mode t per 1 km [kg km^{-1}]
$HD_{sc,ts,g}$	hydrogen demand by grid point g during time period ts for scenario sc [kg d^{-1}]
$InRate$	increasing rate coefficient
LUT_t	load/unload time for transportation mode t [h]
LR	learning rate taking into account cost reduction of facilities as experience accumulates with time
MA_t	transportation mode t availability [h]
$MaxHF_{t,f}$/ $MinHF_{t,f}$,	min/max product flow rate [kg d^{-1}]
$MaxPCap_{p,h}$/ $MinPCap_{p,h}$	max/min production capacity for hydrogen production facility p size h[kg d^{-1}]
$MaxSCap_{s,f}$/ $MinSCap_{s,f}$	max/min capacity of storage facility s for holding hydrogen in the from f [kg]
ME_t	maintenance cost for transportation mode t [\$]
$NetIn$	average income per one household [\$ d^{-1}].
NP	number of time period
OP	operating period [d y^{-1}]
$PCC_{p,h,f}$	capital cost of facility p size h, producing hydrogen in form f [\$ d^{-1}]
$POC_{p,h,f}$	hydrogen production cost in form f at facility p size h [\$ d^{-1}]
$PN_{sc,ts,g}$	population at the grid point g during time period ts and scenario sc
$SCC_{s,f}$	capital cost for storage facility s holding hydrogen in the form f [\$]
$SOC_{s,f}$	operating cost to store 1 kg of hydrogen in the from f inside of storage facility s [\$ kg^{-1} d^{-1}]
Tax_{ts}	tax for kg CO_2 emissions for time period ts [\$ kg^{-1}]
$TCap_{t,f}$	capacity of transportation mode t to distribute produced hydrogen in form f [kg]
$TCC_{f,t}$	capital cost of transport mode t for distribution hydrogen in the form f [\$]
TT	time use of passenger transport by one household [% d^{-1}]
Greek letters	
$\alpha_{e,p,h}$	the ratio between energy sources e consumption for production facility p size h to produce 1 kg [unit e kg^{-1} H_2]
ρ_{sc}	scenario probability [%]
γ_{ts}	FCEVs penetration rate at time period ts[%]
τ	total product storage period [d]

Appendix B.

Table B.1

Parameters used to estimate the capital and unit production costs of hydrogen production technologies.

Parameters	Size	Steam reforming LH	Steam reforming CH	Coal gasification LH	Coal gasification CH	Electrolysis LH	Electrolysis CH	Biomass gasification LH	Biomass gasification CH
Fuel required per H_2 generated unit kg^{-1} H_2	S	4.02	4.02	-	-	47.6	47.6	-	-
	M	3.34	3.34	5.64	5.64	47.6	47.6	18.43	18.43
	L	3.16	3.16	5.44	5.44	47.6	47.6	11.26	11.26
CO_2 produced kg kg^{-1} H_2		17.4	10.3	30.3	19	0.9	0.9	32.1	25.4
Facility capital cost (Mio \$)	S	11.3	8.1	-	-	18.9	16.4	-	-
	M	169.2	121.1	260.6	175.5	284.3	245.7	285.1	227.2
	L	541.5	387.5	833.6	561.5	909.6	786.1	912.0	727.0
Unit production cost (\$ kg^{-1})	S	2.57	1.41	-	-	5.80	4.69	-	-
	M	2.47	1.32	2.55	1.24	5.80	4.69	3.40	2.20
	L	2.45	1.29	2.54	1.23	5.80	4.69	3.04	1.84

where S referred to as small (up to 10 t H_2 d^{-1}), M - medium (up to 150 t H_2 d^{-1}), and L - large (up to 480 t H_2 d^{-1}) maximum production capacity, unit for steam methane reforming, biomass and coal gasification in kg, for water electrolysis in kWh

Table B.2

Parameters used to estimate the capital and operating costs of transportation modes

Transpiration mode	Tanker truck	Tube trailer	Railway tank car	Railway tube car
Capacity (kg $trip^{-1}$)	4082	181	9072	454
CO_2 produced kg km^{-1}	1.05		0.18	
Total cost (\$)	500000	250000	500000	300000
Fuel economy (km $unit^{-1*}$)	2.85		1.133	
Fuel price (\$ $unit^{-1*}$)	1.22		0.07	

*unit for truck and trailer in l, for railway car in kWh

Table B.3

Parameters used to estimate the capital and unit storage costs of hydrogen storage facilities

Storage type	Super-insulated spherical tanks	Pressurized cylindrical vessel
Product form	LH	CH
Capacity (kg)	540 000	540 000
CO_2 produced kg kg^{-1} H_2	5.4	10
Storage capital cost (M \$)	122	1894
Unit storage cost (\$ kg^{-1} d^{-1})	0,005	0,076

Table B.4

Local hydrogen demand for the 2030

German region	Grid point, g	Hydrogen demand, ts (ton d^{-1}) 2026	2032	2038	2044	2050
Baden-Wurttemberg	Stuttgart	197.18	348.65	500.72	650.83	796.16
Bavaria	Munich	234.74	415.95	596.98	774.19	945.14
Berlin	Berlin	66.67	119.29	173.40	228.62	283.91
Brandenburg	Potsdam	43.38	74.62	103.59	129.67	152.90
Bremen	Bremen	11.86	20.77	29.68	38.62	47.30
Hamburg	Hamburg	33.24	59.36	86.38	114.03	141.45
Hesse	Frankfurt	110.73	194.73	278.44	360.85	440.28
Mecklenburg-Vorpommern	Rostock	138.98	242.13	342.54	438.61	529.10
Lower Saxony	Hannover	27.22	46.32	64.12	80.39	94.84
North Rhine-Westphalia	Cologne	313.38	547.03	777.23	1000.37	1212.12
Rhineland-Palatinate	Mainz	70.85	123.35	174.43	222.98	268.44
Saarland	Saarbrucken	16.73	28.63	39.85	50.17	59.53
Saxony	Dresden	70.48	121.27	169.98	216.58	260.64
Saxony-Anhalt	Halle	36.48	61.13	83.78	104.47	122.85
Schleswig-Holstein	Kiel	50.93	89.07	125.83	160.40	192.64
Thuringia	Erfurt	36.16	61.25	84.67	106.41	126.25

Table B.5

Initial availability of energy sources

German region	Grid point, g	Primary energy source, e

		Biomass (ton d^{-1})	Coal (ton d^{-1})	Natural gas (ton d^{-1})	Renewable energy source (GWh d^{-1})
Baden-Wurttemberg	Stuttgart	1.99	0.00	0.00	25.85
Bavaria	Munich	4.62	0.00	0.00	61.50
Berlin	Berlin	0.00	0.00	0.00	0.34
Brandenburg	Potsdam	1.92	95890.41	0.00	55.73
Bremen	Bremen	0.00	0.00	0.00	1.70
Hamburg	Hamburg	0.00	0.00	0.00	0.59
Hesse	Frankfurt	1.13	0.00	0.00	16.43
Mecklenburg-Vorpommern	Rostock	4.39	0.00	0.00	32.51
Lower Saxony	Hannover	5.34	0.00	0.00	112.46
North Rhine-Westphalia	Cologne	2.19	293041.10	0.00	46.47
Rhineland-Palatinate	Mainz	0.63	0.00	0.00	29.67
Saarland	Saarbrucken	0.06	0.00	0.00	3.81
Saxony	Dresden	2.46	95890.41	0.00	15.58
Saxony-Anhalt	Halle	3.07	26027.40	0.00	42.32
Schleswig-Holstein	Kiel	2.91	0.00	0.00	47.50
Thuringia	Erfurt	2.26	0.00	0.00	14.38

Table B.6

Results of Configuration 1

Production stage

Time period, ts	Grid point, g	Type of technology, p	Size, h	Form, f	Number
1	Stuttgart	Steam methane reforming	Large	Liquid	1
1	Munich	Steam methane reforming	Large	Liquid	1
1	Berlin	Steam methane reforming	Large	Liquid	1
1	Rostock	Steam methane reforming	Large	Liquid	1
1	Cologne	Steam methane reforming	Large	Liquid	2
1	Mainz	Steam methane reforming	Large	Liquid	1
1	Dresden	Steam methane reforming	Large	Liquid	1
2	Stuttgart	Steam methane reforming	Large	Liquid	1
2	Munich	Steam methane reforming	Large	Liquid	2
2	Rostock	Steam methane reforming	Large	Liquid	1
2	Cologne	Steam methane reforming	Large	Liquid	2
2	Mainz	Steam methane reforming	Large	Liquid	1
3	Frankfurt	Steam methane reforming	Large	Liquid	1
3	Kiel	Steam methane reforming	Large	Liquid	1
3	Erfurt	Steam methane reforming	Large	Liquid	1

Storage stage

Time period, ts	Grid point, g	Type of technology, s	Form, f	Number
1	Stuttgart	Super-insulated spherical tanks	Liquid	23
1	Munich	Super-insulated spherical tanks	Liquid	27
1	Berlin	Super-insulated spherical tanks	Liquid	8
1	Potsdam	Super-insulated spherical tanks	Liquid	5
1	Bremen	Super-insulated spherical tanks	Liquid	2
1	Hamburg	Super-insulated spherical tanks	Liquid	4
1	Frankfurt	Super-insulated spherical tanks	Liquid	13
1	Rostock	Super-insulated spherical tanks	Liquid	15
1	Hannover	Super-insulated spherical tanks	Liquid	3
1	Cologne	Super-insulated spherical tanks	Liquid	34
1	Mainz	Super-insulated spherical tanks	Liquid	8
1	Saarbrucken	Super-insulated spherical tanks	Liquid	2
1	Dresden	Super-insulated spherical tanks	Liquid	8
1	Halle	Super-insulated spherical tanks	Liquid	4
1	Kiel	Super-insulated spherical tanks	Liquid	6
1	Erfurt	Super-insulated spherical tanks	Liquid	4

Transportation stage

Time period, ts	Grid point. g	Type of technology, t	Form, f	Number
1	Stuttgart	Railway tank car	Liquid	4
1	Munich	Railway tank car	Liquid	9
1	Berlin	Railway tank car	Liquid	11

1	Rostock	Railway tank car	Liquid	22
1	Cologne	Railway tank car	Liquid	10
1	Mainz	Railway tank car	Liquid	13
1	Dresden	Railway tank car	Liquid	16
1	Kiel	Railway tank car	Liquid	3
1	Erfurt	Railway tank car	Liquid	12
2	Stuttgart	Railway tank car	Liquid	7
2	Munich	Tanker truck	Liquid	17
2	Berlin	Railway tank car	Liquid	4
2	Cologne	Railway tank car	Liquid	8
2	Mainz	Railway tank car	Liquid	1
2	Dresden	Railway tank car	Liquid	3
2	Kiel	Railway tank car	Liquid	5
3	Munich	Railway tank car	Liquid	4
3	Frankfurt	Railway tank car	Liquid	5
3	Rostock	Railway tank car	Liquid	2
3	Cologne	Tanker truck	Liquid	32
3	Mainz	Railway tank car	Liquid	3
3	Dresden	Railway tank car	Liquid	2
3	Kiel	Railway tank car	Liquid	4
3	Erfurt	Railway tank car	Liquid	2
4	Stuttgart	Railway tank car	Liquid	3
4	Munich	Railway tank car	Liquid	1
4	Frankfurt	Railway tank car	Liquid	2
4	Rostock	Railway tank car	Liquid	3
4	Mainz	Railway tank car	Liquid	11
4	Erfurt	Railway tank car	Liquid	1
5	Rostock	Railway tank car	Liquid	2
5	Cologne	Railway tank car	Liquid	2
5	Dresden	Railway tank car	Liquid	2
5	Erfurt	Railway tank car	Liquid	1

Summary	
Energy Distribution and Purchase Cost M$ d^{-1}	$4.71
Production Capital Cost M$ d^{-1}	$0.55
Production Operating Cost M$ d^{-1}	$13.04
Storage Capital Cost M$ d^{-1}	$1.13
Storage Operating Cost M$ d^{-1}	$0.03
Transportation Capital Cost M$ d^{-1}	$0.01
Transportation Operating Cost M$ d^{-1}	$0.09
CO_2 fee M$ d^{-1}	$7.69
Penalty $ d^{-1}	$0.00
Global warming potential 10ˆ3 t CO_2 d^{-1}	121.43
Total Cost M$ d^{-1}	$27.25

Table B.7

Results of Configuration 2

Production stage					
Time period, ts	**Grid point, g**	**Type of technology, p**	**Size, h**	**Form, f**	**Number**
1	Stuttgart	Water electrolysis	Large	Liquid	1
1	Munich	Water electrolysis	Large	Liquid	1
1	Rostock	Water electrolysis	Large	Liquid	1
1	Cologne	Water electrolysis	Large	Liquid	1
1	Mainz	Water electrolysis	Large	Liquid	2
1	Dresden	Water electrolysis	Large	Liquid	1
2	Stuttgart	Water electrolysis	Large	Liquid	1
2	Munich	Water electrolysis	Large	Liquid	2
2	Berlin	Water electrolysis	Large	Liquid	1
2	Potsdam	Water electrolysis	Large	Liquid	1
2	Rostock	Water electrolysis	Large	Liquid	1
2	Hannover	Water electrolysis	Large	Liquid	1
2	Cologne	Water electrolysis	Large	Liquid	1
2	Kiel	Water electrolysis	Large	Liquid	1

2	Erfurt	Water electrolysis	Large	Liquid	1
3	Hannover	Water electrolysis	Large	Liquid	1

Storage stage

Time period, ts	Grid point, g	Type of technology, s	Form, f	Number
1	Stuttgart	Super-insulated spherical tanks	Liquid	23
1	Munich	Super-insulated spherical tanks	Liquid	27
1	Berlin	Super-insulated spherical tanks	Liquid	8
1	Potsdam	Super-insulated spherical tanks	Liquid	5
1	Bremen	Super-insulated spherical tanks	Liquid	2
1	Hamburg	Super-insulated spherical tanks	Liquid	4
1	Frankfurt	Super-insulated spherical tanks	Liquid	13
1	Rostock	Super-insulated spherical tanks	Liquid	15
1	Hannover	Super-insulated spherical tanks	Liquid	3
1	Cologne	Super-insulated spherical tanks	Liquid	34
1	Mainz	Super-insulated spherical tanks	Liquid	8
1	Saarbrucken	Super-insulated spherical tanks	Liquid	2
1	Dresden	Super-insulated spherical tanks	Liquid	8
1	Halle	Super-insulated spherical tanks	Liquid	4
1	Kiel	Super-insulated spherical tanks	Liquid	6
1	Erfurt	Super-insulated spherical tanks	Liquid	4

Transportation stage

Time period, ts	Grid point ,g	Type of technology, t	Form, f	Number
1	Stuttgart	Railway tank car	Liquid	4
1	Munich	Railway tank car	Liquid	6
1	Berlin	Railway tank car	Liquid	6
1	Potsdam	Railway tank car	Liquid	11
1	Rostock	Railway tank car	Liquid	9
1	Hannover	Railway tank car	Liquid	4
1	Cologne	Railway tank car	Liquid	5
1	Mainz	Railway tank car	Liquid	26
1	Dresden	Railway tank car	Liquid	15
1	Erfurt	Railway tank car	Liquid	2
2	Stuttgart	Railway tank car	Liquid	10
2	Munich	Railway tank car	Liquid	8
2	Berlin	Railway tank car	Liquid	2
2	Potsdam	Railway tank car	Liquid	3
2	Rostock	Railway tank car	Liquid	3
2	Hannover	Railway tank car	Liquid	52
2	Cologne	Railway tank car	Liquid	2
2	Mainz	Railway tank car	Liquid	8
2	Kiel	Railway tank car	Liquid	6
2	Erfurt	Railway tank car	Liquid	7
3	Potsdam	Railway tank car	Liquid	2
3	Rostock	Railway tank car	Liquid	5
3	Mainz	Railway tank car	Liquid	1
3	Kiel	Railway tank car	Liquid	3
3	Erfurt	Railway tank car	Liquid	4
4	Munich	Tanker truck	Liquid	16
4	Munich	Railway tank car	Liquid	1
4	Cologne	Railway tank car	Liquid	7
4	Mainz	Railway tank car	Liquid	3
4	Kiel	Railway tank car	Liquid	2
4	Erfurt	Railway tank car	Liquid	3
5	Munich	Tanker truck	Liquid	1
5	Berlin	Railway tank car	Liquid	2
5	Potsdam	Railway tank car	Liquid	6
5	Hannover	Railway tank car	Liquid	2
5	Mainz	Railway tank car	Liquid	2
5	Dresden	Railway tank car	Liquid	10
5	Erfurt	Railway tank car	Liquid	11

Summary	
Energy Distribution and Purchase Cost M$ d^{-1}	$16.54
Production Capital Cost M$ d^{-1}	$0.93
Production Operating Cost M$ d^{-1}	$29.68
Storage Capital Cost M$ d^{-1}	$1.13
Storage Operating Cost M$ d^{-1}	$0.03
Transportation Capital Cost M$ d^{-1}	$0.01
Transportation Operating Cost M$ d^{-1}	$0.11
CO_2 fee M$ d^{-1}	$2.13
Penalty $ d^{-1}	$0.00
Global warming potential 10ˆ3 t CO_2 d^{-1}	33.56
Total Cost M$ d^{-1}	$50.55