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# Exploring supply chain design and expansion planning of China's green ammonia production with an optimization-based simulation approach

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## HIGHLIGHTS

- The $H_2$-based energy transition in China's ammonia industry is explored.
- A hybrid approach for green ammonia supply chain design and planning is proposed.
- The cost of green ammonia will be at least twice that of the current level.
- Electricity price and expenses in electrolysers are key impacts to the total cost.
- Storing and selling by-product oxygen can partly reduce the total cost.

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## ABSTRACT

Green ammonia production as an important application for propelling the upcoming hydrogen economy has not been paid much attention by China, the world's largest ammonia producer. As a result, related studies are limited. This paper explores potential supply chain design and planning strategies of green ammonia production in the next decade of China with a case study in Inner Mongolia. A hybrid optimization-based simulation approach is applied, considering traditional optimization approaches are insufficient to address uncertainties and dynamics in a long-term energy transition. Results show that the production cost of green ammonia will be at least twice that of the current level due to higher costs of hydrogen supply. Production accounts for the largest share of the total expense of green hydrogen (~80 %). The decline of electricity and electrolyser prices are key in driving down the overall costs. In addition, by-product oxygen is also considered in the model to assess its economic benefits. We found that by-product oxygen sales could partly reduce the total expense of green hydrogen (~12 % at a price of USD 85/t), but it also should be noted that the volatile price of oxygen may pose uncertainties and risks to the effectiveness of the offset. Since the case study may represent the favourable conditions in China due to the abundant renewable energy resources and large-scale ammonia industry in this region, we propose to take a moderate step towards green ammonia production, and policies should be focused on reducing the electricity price and capital investments in

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green hydrogen production. We assume the findings and implications are informative to planning future green ammonia production in China.


## Introduction

### *The role of ammonia industry in China's hydrogen-based energy transition*

A key challenge today is how to decarbonize fossil fuel-based energy systems as they are increasingly struggling to tackle climate change [1]. As such, the need for an energy transition is well understood, and hydrogen has been assumed as a powerful enabler of the future energy transition [2]. With the concept of 'Power to Gas' (P2G), hydrogen produced from renewable energy sources, also called green hydrogen, can help bring about a clean, secure and sustainable energy future [3].

Producing green hydrogen is still costly at the moment, however. Moreover, shipping and storing it make it more expensive [3]. Overall costs should be brought down by scaling up production of green hydrogen [3]. Strategies and pathways towards a future hydrogen society vary by country. China sees fuel cell vehicles (FCVs) can help to decarbonize transportation, and propel the upcoming hydrogen economy [3,4]. Multiple obstacles stand in the way, however, such as the high cost of FCVs and the infrastructure required [5,6].

Recently, many organizations look to the industry as nowadays hydrogen use is dominated by industrial applications [7,8]. Ammonia production is seen as an opportunity to achieve sufficient green hydrogen demand since it consumes 43 % of global hydrogen demand and the conversion from hydrogen to ammonia is a well-established technology [9]. Moreover, the current fossil fuel-based production process consumes approximately 2 % of worldwide fossil energy and generates over 420 million tons of $CO_2$ annually [10]. Energy transition by the use of green ammonia can tackle energy challenges and offers enormous social and environmental benefits [10]. As a result, it has received much attention in the world. For example, Europe plans to scale up green ammonia production capacity to 1 million ton per year from 2020 [11]. China is the world's largest ammonia producer, presenting 40 % of global ammonia production capacity and consuming about 45 % of hydrogen in domestic China [12,13]. However, green ammonia production has not been well researched and supported on a large scale by the Chinese government [4].

Hence, techno-economic assessment of green ammonia production becomes an essential activity with the purpose of finding cost-effective and sustainable strategies for the transition to future green ammonia industry. A focus on green supply chain (i.e. the concept of integrating green practices into supply chain operations to enhance social and environmental benefits) is of critical importance since energy systems are essentially a supply chain comprising of fuels, technologies, infrastructures, etc., and a better understanding of future green supply chains helps to explore and discuss how to enable the development of future sustainable energy systems [1,14].

### *Techno-economic analysis of green ammonia production*

Studies regarding techno-economic analysis of green ammonia production basically comprise of two groups, including production process and supply chains of green ammonia.

In the aspect of production process, studies are focused on evaluating performance of ammonia production processes and operations. For example, Jain et al. proposed a new route for ammonia synthesis using hydrolysis of nitride [15]. Chen et al. investigated the design of an ammonia synthesis system for thermochemical energy storage [16]. Wang et al. proposed and examined an ammonia-based energy storage system [17]. Al-Zareer et al. proposed and evaluated a low-temperature ammonia production reactor [18]. Yuksel et al. proposed a novel multi-generation plant with hydrogen and ammonia produced [19]. Reese et al. proposed a method for assessing performance of future small scale, distributed ammonia plants [20].

Studies regarding supply chains are conducted on a macro level, that aim to explore the potential of incorporating green ammonia production in future ammonia industry. Recent works regarding green ammonia production in China in this aspect has not drawn much attention of academia. Most recent works are focused on discussing the upcoming hydrogen economy and FCVs applications (e.g. see literature [21–25]). Outside of China, related studies have been performed. For example, Zhang et al. studied techno-economic feasibility of producing green ammonia from biomass and renewable electricity [26]. Guerra et al. analysed investing in a green ammonia production plant, in which green ammonia is produced by solar energy in Chile [27]. Bicer et al. assessed the environment impact of life-cycle ammonia production where hydrogen is produced using various energy sources such as: hydropower, nuclear, biomass, etc. [28]. Demirhan et al. investigated the effects of feedstock types, price and availability on ammonia synthesis processes by incorporating renewable feedstocks [29]. Some works also considered more aspects regarding green ammonia production. For example, Wang et al. investigated economic merits of coupling green ammonia and nitric acid production processes [30]. Cesaro et al. evaluated production costs of green ammonia and electricity costs by applying ammonia as an energy vector up to 2040 [31]. However, recent works are not sufficient, that they are more focused on the production phase of green ammonia, so transporting and storing hydrogen (i.e. gas supply) are not well considered. In other words, the entire supply chain for green ammonia production is not fully studied.

### *Modelling of green ammonia supply chains*

An ammonia production system mainly consists of a gas supply system and an ammonia synthesis system [32]. Ammonia synthesis is an existing and standard process where hydrogen and nitrogen are fed into to produce ammonia, and it will still be applied in future green ammonia production [27]. Therefore, the focus is on how gas supply can be renewable-based (i.e. developing future green hydrogen supply chains).

Research on sustainable supply chain management has emerged in recent years, in which mathematical modelling has been increasingly adopted [33] (e.g. see literature [14,34,35]). Optimization is widely used in recent studies modelling hydrogen supply chains [36]. In many of these works, hydrogen supply chains are designed either for general use or for FCVs applications, but still offer a salutary lesson. For example, Kim et al. presented a mixed integer linear optimization (MILP) optimization model for future hydrogen supply system design in Korea [37]. Brey et al. designed a hydrogen supply chain for hydrogen production, consumption and transport for the transition towards a hydrogen economy in Spain with a multi-objective optimization model [38]. Almansoori et al. studied future hydrogen supply chain design for Germany with a MILP model by taking emission constraints and carbon tax into account [39]. Similar studies are fewer in the aspect of green ammonia supply chains. For example, Palys et al. proposed an ammonia supply chain optimization model that incorporates green ammonia plants into the conventional ammonia supply chains [40]. Smith et al. modelled the near-optimal infrastructure of green ammonia supply chain in Sierra Leone with an iterative optimization method [41]. In general, these works solve the distribution of hydrogen plants, transport, storage infrastructures, etc. for a single period. However, from the energy transition perspective, the formation of future renewable-based energy systems is often long and protracted, usually taking years or decades [42]. Furthermore, these traditional optimization approaches fail to address the uncertainty and complexity of energy systems, especially when the problem size and complexity increase [43].

To address these issues, since simulation is an appropriate tool for addressing practical applicability in energy systems, a combination of simulation and optimization, also called hybrid simulation-optimization (SO), is assumed to be a prospective direction for modelling energy transitions [43,44]. The optimization-based simulation approach is a branch of SO approaches [43]. In contrast to classic optimization models, the optimization process is embedded in a simulation model to address complex interrelations in energy systems over long time horizons. It has been applied in supply chain management. For example, Liu et al. integrated multi-objective optimization and system dynamics simulation for optimizing the structure of a straw-to-electricity supply chain and designing motivational mechanisms [45]. Shaghaygh et al. introduced an recursive optimization-based simulation approach for planning bioenergy and biofuel supply chains [46]. Joao et al. studied wind power expansion planning in North Sea of Europe with myopic optimization models classified as optimization-based simulation approaches [47,48]. One example for planning green ammonia production is done by the work [32], where a Balmorel-VTT model was introduced to simulate power to ammonia in the North Europe in 2050 by scheduling optimal operation of renewable power plants, electrolysers, ammonia storage, etc. on an hourly basis. However, the focus is on operation management of ammonia production, other than long-term supply chain planning. In our literature search, we found that no related approach has been applied to green ammonia supply chain planning with long-term variations and dynamics taken into account. As a result, in this paper, we introduce a hybrid optimization-based simulation model for analysing green ammonia supply chain design and planning at strategic and tactical levels. It leverages the advantages of simulation models by exploring energy transition planning with scenarios, and provides the optimum for each time slot, which helps to improve the reliability of the results.

Besides, since oxygen is a by-product in the electrolysis process, a few studies take account of oxygen in the modelling of a green hydrogen supply system. The recent studies are still not sufficient, however. For example, Kim et al. considered oxygen production in the technical design of hydrogen supply system for Korea [37], but the related economic impact by oxygen is not studied. Kato et al. compared the hydrogen production costs via electrolysis and steam reforming (SMR) with oxygen costs taken into account in the electrolysis process [49]. However, additional investments and operating costs caused by oxygen are not taken into account in the assessment. Hence, the issue of to what extent green hydrogen production can benefit from selling by-product oxygen is not well investigated. In addition, results can also vary according to different infrastructure and oxygen prices applied.

### *Research goal and contribution*

In summary, green hydrogen as a feedstock for ammonia industry use to boost the energy transition towards a hydrogen society in China has not been paid too much attention so far. As a result, the related supply system design and planning are not yet well researched. Beyond China, related studies are focused on the production phase of green ammonia, the entire supply chain including hydrogen supply is not fully considered. Regarding supply chain modelling, traditional optimization methods that are widely used for modelling supply chains are not sufficient to capture the high degrees of variation and complexity in a long-term energy transition process. Besides, results on the economic benefits of by-product oxygen to green hydrogen production are limited in recent studies, and also differ depending on infrastructure and oxygen prices.

This paper aims to explore potential supply chain design and planning strategies for green ammonia production in China in the next decade. The contributions of this paper are as follows:

1) The exploration is conducted with a case study in Inner Mongolia, representative of the favourable conditions in

China in the next decade. Therefore, the findings and implications are informative to planning future green ammonia production in China.

2) A supply chain for green ammonia production is proposed. It covers an entire supply chain ranging from hydrogen production, transport, storage to final ammonia production, other than only focusing on the production phase of green ammonia that most recent works did.
3) A hybrid optimization-based simulation approach is proposed for analysing supply chain design and planning. It helps to deal with uncertainties and dynamics in the energy transition and reveal key drivers affecting the system expansion from a number of contributors, such as: expansion speeds, scales of the economy, learning effects, capital investments, renewable electricity prices, etc. The approach is also applicable for analysing cases beyond China.
4) The sales of by-product oxygen and the related infrastructure design are considered, and the assessment of its complementary value to green hydrogen production is also performed. That also partly examines the possibility of integrating the two industry sectors in the future.

### Paper structure

The remainder of this paper is arranged as follows: details about the hybrid optimization-based simulation approach are introduced in Section Methods. With a case study, Section Application discusses the infrastructure design, economic assessment of the supply chain in each scenario and potential impacts to the future ammonia industry. Following this, a model calibration process is described as well, in which a sensitivity analysis is discussed to examine the effects of uncertain parameters on the final results. Section Discussions and policy implications draws key findings, policy implications, and notes the limitations of this work. Section Conclusions summarizes the work of this paper.

## Methods

### System description

As shown in Fig. 1, we proposed a green ammonia supply chain in which hydrogen is produced and temporarily stored at renewable power plants and later transported by lorry to the ammonia plant for ammonia synthesis. The hydrogen supply system consists of three parts: production, transport and storage.

Wind, solar and biomass as main renewable energy sources are considered for green hydrogen production. Alkaline electrolysers (AECs) and Proton Exchange Membrane electrolysers (PEMECs) as the most mature electrolysers so far are considered and assumed to be installed on the renewable power plants. AECs are mostly applied in China for lower capital investments; PEMECs are rapidly emerging and widely used in Europe and capital costs are expected to decline more rapidly in the future [3,50,51]. Regarding storage, we consider both hydrogen and oxygen storage. Oxygen as a by-product of green hydrogen production is involved in the system to examine its impacts to the system design and overall costs. Besides, although the cost of underground storage is much lower, it is limited by geographical conditions. Hence, in this study we mainly consider two types of aboveground storage solutions - cryotanks and pressure tanks to store liquid and gaseous hydrogen respectively. Storage tanks are installed at power plants to temporarily store hydrogen and oxygen. Although pipeline transport is expected to be a cost-effective long-term choice, road transport is likely to remain the main hydrogen distribution mechanism over the next decade, especially for short-distance transportation due to the flexibility [3]. Tube trailers and liquid tankers are both taken into account as road transport tools for carrying on-site hydrogen (gaseous and liquid respectively) to the ammonia plant, where storage tanks will also be installed to store hydrogen downloaded from lorry. Besides, it is assumed that oxygen will be traded and shipped from power plants by retailers, so transportation of oxygen is not considered in the system. The related techno-economic parameters applied to the supply chain design are listed in Table 1 [3,9,52–56].

### Framework of the hybrid model

The development of the hybrid model referred to the models developed in the works [47,48] for wind power expansion planning. They are classified as simulation models able to capture time-dependent factors in the system expansion that runs iteratively and in each turn the optimization horizon considers the current slot of the entire time period [47]. We further improved the framework to a hybrid model by splitting it into separate simulation and optimization models following the instructions in the work [43].

Fig. 2 shows the framework of the designed hybrid model. To explain: this model simulates the expansion of a green hydrogen supply system on a yearly basis, in which optimization is applied to design the expanded system required per year $n$. The model runs iteratively, starting from the first year and terminating when it hits the end year (i.e. $n = 1, 2, 3 \ldots N$ in Fig. 2).

The penetration rate of the renewable-based system (i.e. $PR(n)$ in Fig. 2) is a time-dependent input of this model, based on which the extent of new installed capacity can be settled per year $n$. Investment costs per unit of production (i.e. $IC(n)$ in Fig. 2) also vary with time, and includes assorted facility ranging from hydrogen production and transport to storage. In addition, the variation of the renewable electricity price (i.e. $EP(n)$ in Fig. 2) during the entire expansion lifetime is also considered.

In each iteration, the model first runs from the simulation model which updates the exogenous and endogenous data to period. In this process, the simulation model calls the optimization model for optimal infrastructure design for the increased expansion to satisfy the renewable hydrogen demand required for each year unless there is no further demand, namely, the system expansion is finished and the capacity of existing fossil fuel-based production system is fully replaced by that of the renewable-based system.

After obtaining techno-economic features of the energy system (i.e. $TEP(n)$ in Fig. 2) from the simulation model, the

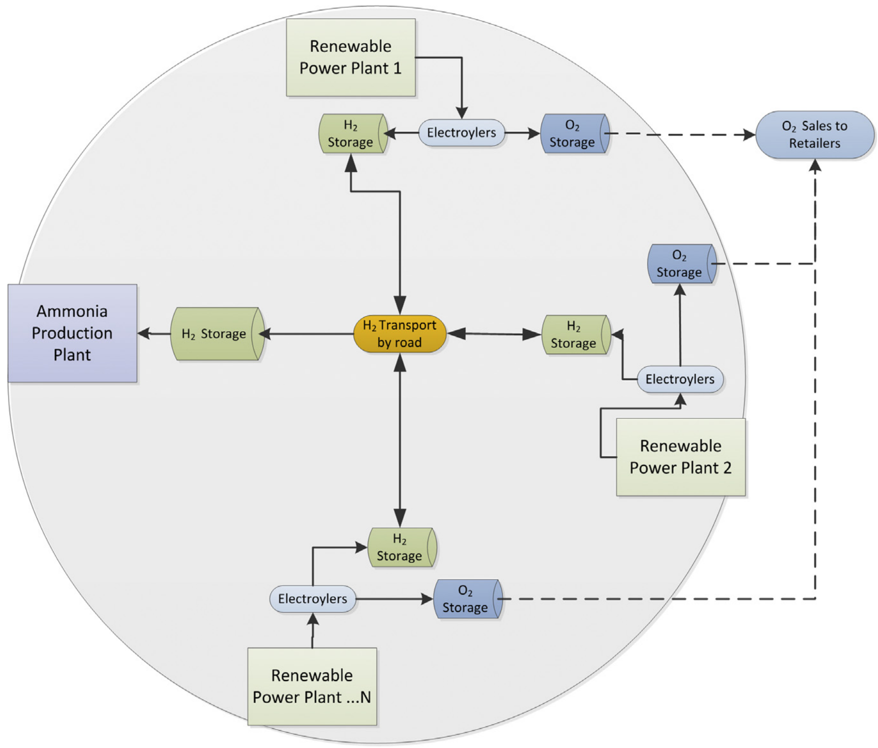


**Fig. 1 – The designed green hydrogen supply system. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)**

**Table 1 – Techno-economic parameters applied to the supply chain design.**

| Parameter | Value | Unit |
|---|---|---|
| Electrical efficiency of AEC | 70 % | dimensionless |
| Electrical efficiency of PEMEC | 60 % | dimensionless |
| Capital cost of AECs (1 MW) | 1265 | USD/KW |
| Capital cost of AECs (5 MW) | 781 | USD/KW |
| Capital cost of AECs (10 MW) | 750 | USD/KW |
| Capital cost of AECs (50 MW) | 682 | USD/KW |
| Capital cost of PEMECs (1 MW) | 1430 | USD/KW |
| Capital cost of PEMECs (5 MW) | 1243 | USD/KW |
| Capital cost of PEMECs (30 MW) | 1034 | USD/KW |
| Capital cost of PEMECs (100 MW) | 770 | USD/KW |
| Annual capital cost decrease rate of AECs | 3.2 % | dimensionless |
| Annual capital cost decrease rate of PEMECs | 4.1 % | dimensionless |
| Transport capacity of tube trailer | 350 | kg |
| Transport capacity of liquid tanker | 4000 | kg |
| Hydrogen residual rate in tube | 20 % | dimensionless |
| Capital cost of tube trailer | 228,571 | USD |
| Capital cost of liquid tanker | 500,000 | USD |
| Annual decrease rate of capital cost of tube trailer | 2.2 % | dimensionless |
| Annual capital cost decrease rate of liquid tanker | 6.5 % | dimensionless |
| Storage capacity of compressed tank | 1000 | cu m |
| Storage capacity of liquid tank | 1000 | cu m |
| Storage pressure of compressed tank | 3 | MPa |
| Capital cost of compressed tank | 1000 | USD/cu m |
| Capital cost of liquid tank | 2500 | USD/cu m |
| Annual capital cost decrease rate of storage tank | 2.1 % | dimensionless |

optimization model does the calculation and returns the infrastructure design for the increased expansion to the simulation model (i.e. *HSD(n)* respectively in Fig. 2). Afterwards, the simulation process continues, during which the designed system expansion will be added to the existing system and techno-economic features will be updated after interactions in the simulation process. The entire infrastructure of the supply system, as well as its hydrogen production volume, economic related results (i.e. *HSS(n)*, *HP(n)*, *HCR(n)* respectively in Fig. 2) in the year *n* will again become inputs for a next year, which will impact the dynamics of the energy system in both technical and economic senses. For example, it ensures that new system infrastructure expansion will continue on the basis of the existing infrastructure of the last year. It makes sense in the situation where there are multiple renewable power plants: instead of choosing to expand on a new power plant at a year *n*, the system expansion will continue at the power plant that was utilised the previous year until the capacity of this power plant is exhausted. This is aligned with the reality that the infrastructure expansion is unlikely to take place in a new location if the selected location is still underused, as the contract is made and some of expenses of hydrogen plant construction are one-off payments.

## Model formulation

### *Optimization model*

A mixed integer linear programming (MILP) optimization model is designed and improved on the basis of previous works [37–39]. Besides, as the model is applied to design the

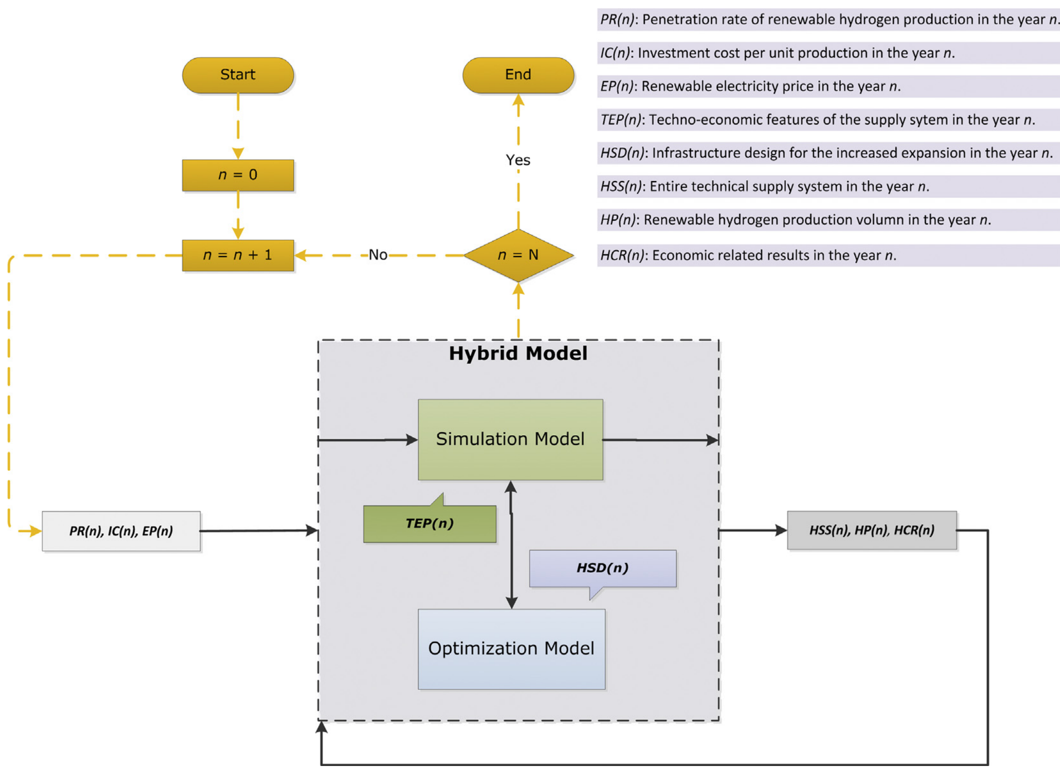


**Fig. 2 – Framework of the hybrid optimization-based simulation model.**

additional system infrastructure required for each year, it should be noted that all the content below refers to the expanded supply system (ESS) rather than the entire supply system of each year. The decision variables, optimization function and constraints are introduced as below.

*Decision variables*. As energy systems are becoming increasingly complex as developments, modelling energy systems requires a reduction of unnecessary level of detail in order to achieve the simplification and the best trade-off between the level in accuracy and complexity [57,58]. As some facilities serve as supplements to main facilities, the quantity of these facilities correlates with that of main facilities. As a result, the size of main facilities in each part of the supply chain form decision variables in the optimization shown in Table 2. Beside this, index parameters of degrees of freedom are summarized in Table 3.

*Objective function*. The objective function shown in Eq. (1) is aimed to minimize the total cost of the ESS per year $n$ consisting of hydrogen production cost ($P^{cost}{}_n$), hydrogen storage cost ($S^{cost}{}_n$), hydrogen transport cost ($T^{cost}{}_n$), oxygen storage cost ($O^{cost}{}_n$) and income from oxygen sales ($O^{rev}{}_n$).

$$min.\ P_n^{cost} + S_n^{cost} + T_n^{cost} + O_n^{cost} - O_n^{rev} \tag{1}$$

The hydrogen production cost given in Eq. (2) comprises expenses relating to electrolysers and miscellaneous expenses including electrical baseline, construction and installation expenses, etc. The electrolyser-related expenses derived from Eqs. (3) and (4) consist of capital investment and operating expenses per year $n$.

**Table 2 – Definition of the decision variables.**

| Notation | Definition |
|---|---|
| $PN_{n,f,e}$ | Number of electrolysers $e$ required at the power plant $f$ in the $n$th year. |
| $T_{n,f,t}$ | Hydrogen distribution rate by transport tools $t$ at the power plant $f$ in the $n$th year. |
| $S_{n,f,s}$ | Hydrogen inventory in storage tanks $s$ at the power plant $f$ in the $n$th year. |
| $S_{n,a,s}$ | Hydrogen inventory in storage tanks $s$ at the ammonia production plant in the $n$th year. |
| $O_{n,f,r}$ | Oxygen inventory in storage tanks $r$ at the power plant $f$ in the $n$th year. |

$$P_n^{cost} = \sum_f \sum_e \left( P_{n,f,e}^{cost} + P_{n,f,e}^{mcost} \right) \tag{2}$$

$$P_{n,f,e}^{cost} = \left( P_{n,e}^{invcost} * P_e^{crf} + P_{n,e}^{optcost} + E_n^{prc} * WH \right) * P_{n,f,e} \tag{3}$$

$$P_{n,f,e} = PN_{n,f,e} * P_e^{cap} \tag{4}$$

The hydrogen storage cost given in Eq. (5) comprises storage cost at each power plant and at the ammonia plant, which includes expenses relating to storage tanks and miscellaneous expenses derived from Eqs. (5) and (6) and Eqs. (7) and (8) respectively. Storage tank-related cost includes annual capital investment and operating expense. Miscellaneous

**Table 3 – Definition of the index parameters.**

| Notation | Index range | Standing value |
|---|---|---|
| $n$ | {1, 2, ..., N} | [Year 1, Year 2, ..., Year N] |
| $a$ | -{1}- | [Ammonia production plant] |
| $f$ | -{1, 2, ..., F}- | [Power plant 1, Power plant 2, ..., Power plant F] |
| $e$ | {1, 2, 3, 4, 5, 6, 7, 8} | [AEC (1 MW), AEC (5 MW), AEC (10 MW), AEC (50 MW), PEMEC (1 MW), PEMEC (5 MW), PEMEC (30 MW), PEMEC (100 MW)] |
| $t$ | {1, 2} | [Tube trailer, Liquid tanker] |
| $s$ | {1, 2} | [Pressure tank, Cryotank] |
| $r$ | {1, 2} | [Pressure tank, Cryotank] |

expenses include installation expense and expenses of other facilities, such as: compressors, pressure regulators, etc. for the compression process and liquefiers, heat exchangers, etc. for the liquefaction process.

$$S_n^{cost} = \sum_f \sum_s \left(S_{n,f,s}^{cost} + S_{n,f,s}^{mcost}\right) + \sum_s \left(S_{n,a,s}^{cost} + S_{n,a,s}^{mcost}\right) \tag{5}$$

$$S_{n,f,s}^{cost} = \left(S_{n,s}^{invcost} * S_s^{crf} + S_{n,s}^{optcost}\right) * SN_{n,f,s} * S_s^{cap} \tag{6}$$

$$SN_{n,f,s} = ceil\left(S_{n,f,s} / S_s^{cap}\right) \tag{7}$$

$$S_{n,a,s}^{cost} = \left(S_{n,s}^{invcost} * S_s^{crf} + S_{n,s}^{optcost}\right) * SN_{n,a,s} * S_s^{cap} \tag{8}$$

$$SN_{n,a,s} = ceil\left(S_{n,a,s} / S_s^{cap}\right) \tag{9}$$

The hydrogen transport cost given in Eq. (10) is a sum of expenses relating to transport tools, which consist of investment expense, fixed operating expense and fuel expense derived from Eq.(11–13).

$$T_n^{cost} = \sum_f \sum_t T_{n,f,t}^{cost} \tag{10}$$

$$T_{n,f,t}^{cost} = \left(T_{n,t}^{invcost} * T_t^{crf} + T_{n,t}^{optcost}\right) * TN_{n,f,t} * T_t^{cap} + T^{fcost} * T_{n,f,t}^{dts} \tag{11}$$

$$TN_{n,f,t} = ceil\left(T_{n,f,t} / T_t^{cap}\right) \tag{12}$$

$$T_{n,f,t}^{dts} = TN_{n,f,t} * D_f * T_{f,t}^{feq} * WD \tag{13}$$

The oxygen storage cost given in Eq. (14) comprises expenses relating to storage tanks and miscellaneous expenses including installation expense, expenses of other facilities, etc. Storage tank-related cost includes annual capital investment and operating expense.

$$O_n^{cost} = \sum_f \sum_r \left(O_{n,f,r}^{cost} + O_{n,f,r}^{mcost}\right) \tag{14}$$

$$O_{n,f,r}^{cost} = \left(O_{n,r}^{invcost} * O_r^{crf} + O_{n,r}^{optcost}\right) * ON_{n,f,r} * O_r^{cap} \tag{15}$$

$$ON_{n,f,r} = ceil\left(O_{n,f,r} / O_r^{cap}\right) \tag{16}$$

Income from oxygen sales given in Eq. (17) is a sum of revenues at each power plant per year $n$. The oxygen production derived from Eq.18 and 19 is calculated on the basis of annual hydrogen production.

$$O_n^{rev} = \sum_f OP_{n,f} * O^{prc} \tag{17}$$

$$OP_{n,f} = HP_{n,f} * CF^{ho} \tag{18}$$

$$HP_{n,f} = \sum_e P_{n,f,e} * CF^{hp} \tag{19}$$

Besides this, the capital recovery factor (CRF) which is applied to calculate annual fixed cost is based on Eq. (20) [59,60].

$$CRF = \frac{dr}{1 - (1 + dr)^{-m}} \tag{20}$$

*Constraints*. The model is subject to a set of constraints. First, the sum of the hydrogen production rate and its surplus capacity from the previous year must meet the incremental demand of year $n$, which is given as follows:

$$\sum_f \left(HP_{n,f} + HP_{n-1,f}\right) - DM_{n-1} \geq DM_n,\ \forall n,f,\ HP_{0,f} = 0,\ DM_{0,f} = 0 \tag{21}$$

The sum of total hydrogen production rate is constrained so as to have no excess to its maximum production rate at each power plant, which is given as follows:

$$0 \leq \sum_n HP_{n,f} \leq HP_f^{max},\ \forall n,f \tag{22}$$

The hydrogen distribution capacity and its surplus capacity from the previous year must meet the hydrogen production rate at each power plant per year $n$, which is given as follows:

$$\sum_t \left(T_{n,f,t} + TN_{n-1,f,t} * T_t^{cap} - T_{n-1,f,t}\right) * T_{f,t}^{feq} \geq HP_{n,f},\ \forall n,f,t,\ T_{0,f,t} = 0,\ TN_{0,f,t} = 0 \tag{23}$$

The hydrogen storage capacity and its surplus capacity from the previous year must at least meet the one-round total distribution capacity from each power plant to the ammonia plant. The constraint is given as follows:

$$\sum_s \left(S_{n,f,s} + SN_{n-1,f,s} * S_s^{cap} - S_{n-1,f,s}\right) \geq \sum_t \left(T_{n,f,t} + TN_{n-1,f,t} * T_t^{cap} - T_{n-1,f,t}\right),\ \forall n,f,s,t,\ S_{0,f,s} = 0,\ SN_{0,f,s} = 0,\ T_{0,f,t} = 0,\ TN_{0,f,t} = 0 \tag{24}$$

Besides this, hydrogen storage capacity at the ammonia plant and its surplus capacity from the previous year must satisfy the hydrogen production in a given storage period per year *n*. The constraint is given as follows:

$$\sum_s \left(S_{n,a,s} + SN_{n-1,a,s} * S_s^{cap} - S_{n-1,a,s}\right) \geq \sum_f HP_{n,f} * S_a^{hsp},\ \forall n,a,f,s,\ S_{0,a,s} = 0,\ SN_{0,a,s} = 0 \tag{25}$$

The oxygen storage capacity and its surplus capacity from the previous year must satisfy the total oxygen production in a given storage period per year *n*. The constraint is given as follows:

$$\sum_r \left(O_{n,f,r} + ON_{n-1,f,r} * O_r^{cap} - O_{n-1,f,r}\right) \geq OP_{n,f} * S_f^{osp},\ \forall n,f,r,\ O_{0,f,r} = 0,\ ON_{0,f,r} = 0 \tag{26}$$

*Simulation model*

We build the simulation model with the concept of System Dynamics (SD), as it is one of the most common and appropriate simulation methods for addressing complex interrelations in energy systems over relatively long time horizons [44]. Our model is applied to simulate the expansion of a green hydrogen supply system in the future on a yearly basis. Fig. 3 shows the causal loop diagram of the simulation model.

To explain: the yearly supply system expansion is influenced by annual expansion rate (i.e. energy transition speed), economies of scale, infrastructure facility price, electricity price, technology learning effect and the existing system infrastructure from last year. The annual growth rate of hydrogen demand is, in other words, the pace of the energy transition which determines the installed infrastructure capacity for each year. The installed capacity positively correlates with the quantity and size of facility to be procured. The unit cost of infrastructure facility is brought down when larger quantity or size of facility is required, i.e. the emergence of economies of scale [61]. Meanwhile, expense for facility procurement is also driven down by lower price of facility of the same type. Manufacturing process is assumed to be improved as production increases, which reinforces productivity and ultimately leads to a decline in capital and process expenses —i.e. the technology learning effect occurs with time and production volume [62].

Besides, as mentioned above, with these techno-economic features and existing infrastructure, new infrastructure design will be achieved in the optimization model, and the expanded system will be integrated to the existing hydrogen supply system until the penetration rate reaches 100 %, namely renewable-based production fully replaces the fossil-fuel based production. Afterwards, no system expansion is required, but the production process will still be improved until the simulation process is complete.

## Application

### *Selection of a case study*

To study future green ammonia production in China, the years 2020–2030 were set as the timeline and an ammonia producer in the Inner Mongolia region was selected. We made this selection because there are many chemical enterprises including

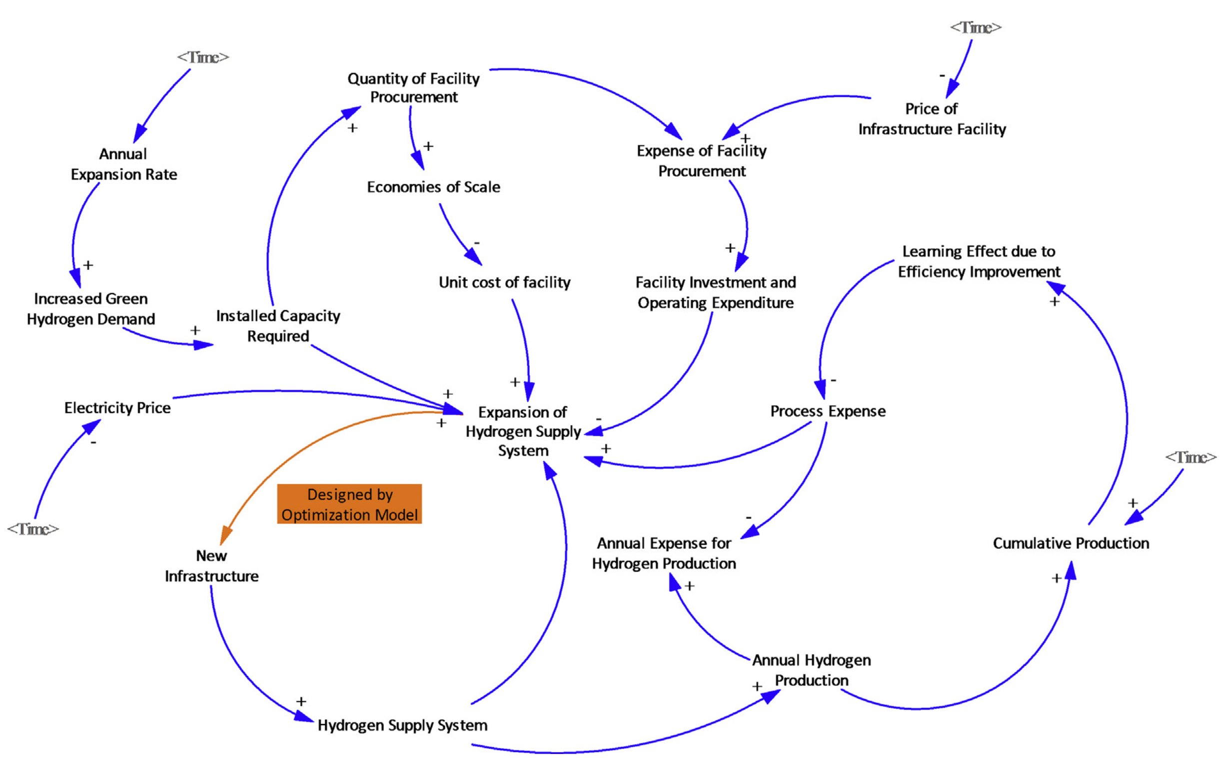


**Fig. 3 – Causal loop diagram of the simulation model.**

ammonia manufacturers in this region due to the abundant fossil fuel energy resources [63]. In addition, this region is rich in renewable energy resources [63]. The generation costs of wind and solar power are the lowest in China [64]. These factors make Inner Mongolia an ideal region for the energy transition in the ammonia industry to start in. Besides, it should be noted that our purpose is to explore potential supply chain design and transition pathways with a typical case study rather than developing a supply chain for a specific enterprise. Hence, we chose a medium-sized ammonia producer in this area in order to obtain the most average conditions in the next decade.

The following assumptions apply. 1) Renewable power plants in this area are able to supply electricity for green hydrogen production. 2) The renewable electricity price decreases at the same rate as its generation cost, and is expected to show a linear decrease in the next decade. 3) In order to avoid higher capital costs of electrolysers, it is assumed to use base-load power of wind and solar energy with a 70 % feed factor, and import grid electricity as back-up power to ensure a reliable power supply for electrolysis. 4) We assume a 2 % learning rate due to specialization and efficiency improvement. This is because learning curves in renewable hydrogen production are not yet well observed [65], and learning rates observed in other industrial processes (which basically range from 5 to 25 % [66]) are caused by the holistic effects of learning, specialization, scale, policy changes, etc. [67,68]. For example, the learning rate observed for natural gas production in the 1980s is around 14 %; off-shore wind power generation is around 12 % in its initial stage [67]. Therefore, we assume that the effects of learning and specialization will not be too high.

**Table 4 – Techno-economic parameters of the case study.**

| Parameter | Value | Unit |
|---|---|---|
| Ammonia production capacity | 300,000 | t/y |
| Operating rate | 95 % | dimensionless |
| Annual operating hours | 8160 | h/y |
| Discount rate | 8 % | dimensionless |
| Learning rate | 2 % | dimensionless |
| Utilization hours of wind power | 2780 | h/y |
| Utilization hours of solar power | 1520 | h/y |
| Utilization hours of biomass power | 4895 | h/y |
| Price of wind power in 2020 | 50 | USD/MWh |
| Price of solar power in 2020 | 71 | USD/MWh |
| Price of biomass power in 2020 | 91 | USD/MWh |
| Price of back-up power from grids | 42 | USD/MWh |
| Feed factor of wind and solar power | 70 % | dimensionless |
| Cost decrease of wind power in the next decade | 15 % | dimensionless |
| Cost decrease of solar power in the next decade | 20 % | dimensionless |
| Cost decrease of biomass power in the next decade | 20 % | dimensionless |
| Oxygen price | 85 | USD/t |
| Hydrogen storage period at the ammonia plant | 2 | d |
| Oxygen storage period at power plants | 1 | d |
| Extra energy for heating and pressurization for ammonia production | 0.6 | MWh/t |
| Costs of catalyst, chemicals for ammonia production | 2.9 | USD/t |

Details about the parameters used in this case study are listed in Table 4 and are based on literature [69–76]. The oxygen and hydrogen storage periods are design parameters for this case, and we set them as 1 and 2 days respectively due to the significant production capacities for both. Besides, Table 5 summarizes the available renewable power plants close to the ammonia plant selected [77,78].

### *Scenario definitions*

To observe the difference between expansion modes, we set up scenarios shown in Table 6 representing four typical planning strategies, in which the starting year and speed of the expansion are separate. Scenario A concerns a fast mode in terms of the implementation of green supply chain, assuming that a green hydrogen supply system is immediately implemented in 2020 and is 100 % available from 2021. Scenario B concerns a slow mode, assuming that a gradual step is made in terms of implementing the energy transition starting from 2020 and completing in 2028 with a 10 % annual expansion rate. Scenario C concerns a faster mode, assuming that the energy transition takes place with a fast step starting from 2020 and ready in 2024 and a 20 % annual expansion rate. Similar to Scenario C, the annual expansion rate of Scenario D is 20 %, but it starts from a later stage, which is 2025, and completes in 2029.

### *Results*

As mentioned above, the hybrid model is essentially a simulation model that runs recursively with optimization model embedded to solve the design of the supply system in each time slot of an expansion. The model is implemented in Matlab to enable the high-level analysis required. Intlinprog solver of Matlab is embedded in the optimization model to help solve the optimization problems, and the simulation model is fully compiled by our own efforts. In contrast with conventional multi-period optimization models (e.g. dynamic programming models), the purpose is not to achieve a global optimal solution in an entire expansion period, but to obtain the performance during the expansion and used for scenario-based analysis.

In addition, the advantages over the conventional models comes from two aspects. First, it dramatically reduces the computational complexity, which sometimes is intractable for conventional models to deal with. It especially helps when the problem size and complexity increase. In this case study, the numbers of decision variables and constraints of the

**Table 5 – Details of available renewable power plants in the area.**

| Power plant | Renewable energy | Installed capacity (MW) | Distance (km) |
|---|---|---|---|
| Plant 1 | Biomass | 2.4 | 38 |
| Plant 2 | Wind | 99 | 93 |
| Plant 3 | Solar | 120 | 105 |
| Plant 4 | Wind | 587.5 | 116 |
| Plant 5 | Wind | 99 | 117 |
| Plant 6 | Wind | 400 | 151 |
| Plant 7 | Wind | 49.5 | 240 |

**Table 6 – Details of scenario definitions.**

| Scenario | Mode | Start year of the system expansion | End year of the system expansion | Increased penetration rate per year |
|---|---|---|---|---|
| A | Fast | 2020 | 2020 | 100 % |
| B | Slow | 2020 | 2028 | 10 % |
| C | Medium | 2020 | 2024 | 20 % |
| D | Medium | 2025 | 2029 | 20 % |

optimization model in each iteration vary with time but are below 100 and 30 respectively. The execution time of the optimization per iteration ranges from 0.2 to 2.3 s, and total execution time of the simulation for each scenario ranges from 3.7 to 5.1 s. More importantly, the objective function and constraints in the optimization model can be adjusted and updated in each iteration of a simulation process to address the dynamics and uncertainties in the supply chain expansion, which conventional models fail to tackle.

Besides, technical and economic assessments are discussed as follows based on basic data obtained including: 1) Number of each main facility for hydrogen production, transport and storage at each power plant for each year; 2) hydrogen production rate, transport flow rate, and storage inventory at each power plant for each year; 3) total expenses in hydrogen production, transport and storage at each power plant for each year; 4) Number of hydrogen storage tanks, storage inventory and related expenses at the ammonia plant for each year; 5) Number of oxygen storage tanks, oxygen production and storage capacities at each power plant for each year; 6) expenses in oxygen production and storage and oxygen sales income at each power plant for each year.

*Technical design*

Table 7 sets out the infrastructure design after the expansion for Scenario A, B, C and D respectively. The figures in the first column are the sequence numbers of the power plants that have been selected, and AM represents the ammonia plant. The results show that biomass and solar power plants are not selected in all the scenarios when wind power plants are able to fully support the production, although these plants are closer to the ammonia plants than most of the others. This is because the wind power price will still be lower than that of solar and biomass energy in the next decade.

Although the capital costs of PEMECs decrease faster, AECs are selected in all scenarios due to their higher electrical efficiency and lower unit cost. Regarding hydrogen storage, pressure tanks are selected in all scenarios rather than liquid tanks, indicating that gaseous storage will still be the primary hydrogen storage approach in the near future. As indicated in some studies (e.g. literature [9,53,54]) that although liquid hydrogen storage can improve the energy density, facilities required for liquefaction are much more costly, and liquefaction requires more than ten times the energy the compression process consumes. This is also the case for oxygen storage, as gaseous storage is more cost-effective than liquid storage. The pressure tanks required for oxygen storage are far fewer than the hydrogen tanks due to the storage period for oxygen being shorter than that of hydrogen stored at the ammonia plant, and its density is higher than that of hydrogen. Tube trailers are selected for hydrogen transport rather than liquid tankers, aligned with the view in the work [9] that compressed hydrogen offers the lowest cost for short-distance transport.

Larger size AECs are selected in Scenario A, which results in lower unit investment costs; Scenario A shows greater benefit from economies of scale. Results in Scenarios B, C and D are final outputs after multi-year expansions. Scenario C and D present the same results partly because of the same penetration rate assigned. This also indicates that the infrastructure of electrolysis by AECs, gaseous transport and storage are still economically preferable even in the second half of next decade. Besides, the system expansion ends up with the same results for B and C (or B and D) in terms of selected power plants and aggregate capacity at each plant, although the number of a specific facility may differ.

*Economic assessment*

*Decrease of unit cost of hydrogen*. Fig. 4 shows the unit costs of hydrogen from 2020 to 2030, including by-product oxygen sales at a price of 85 USD/t. As expected, the costs decline in all scenarios. However, the trajectories are different for each scenario.

As Scenario A has the largest cost advantages from the economies of scale, the unit cost starts at 3.95 USD/kg, which is the lowest level for 2020. Then it experiences a modest decline due to the technology learning effect, and ends up with about 7.9 % reduction in total. In Scenario B, the unit cost starts at 4.30 USD/kg, the highest level – for 2020, and is about USD 0.9 lower at 2030, which is the largest decrease (about 22.9 %) in all scenarios.

In Scenario C, the unit cost starts at 4.06 USD/kg in 2020, which is very close to that of in Scenario A, indicating that the impact exerted on the cost decline by the economies of scale is not obvious when the annual penetration rate is above 20 %. Cost experiences a sharp decline until 2024, which is similar to that in Scenario B. After 2024, it turns into a gradual decrease and ultimately ends up having decreased by 16.5 %. In Scenario D the unit cost starts at 3.70 USD/kg in 2025, which is much lower than the unit cost in 2020. Then it has a sharper decrease than that of in other scenarios mainly due to cheaper electricity and lower investment costs. It ends at 3.17 USD/kg, which is also the lowest level in all scenarios. This indicates that the hydrogen cost could be further driven down by a reduction in electricity and facility prices in the next decade.

*Levelized cost of hydrogen*. To further compare the difference between different planning strategies, the levelized cost of hydrogen (LCOH) in each scenario is calculated. This is loosely regarded as the long-term average unit cost of hydrogen [60].

Fig. 5 shows LCOHs and total hydrogen production volumes under different scenarios. Two types of LCOH are calculated: one is the LCOH with oxygen-related expenses and incomes excluded (the blue columns); the other one is the LCOH with oxygen-related items considered (the red columns). As demonstrated, Scenario A has the largest hydrogen production volume in the next decade (about 583.6 kt), followed by Scenario C (about 477.8 kt) and B (about 345.4 kt). As hydrogen

**Table 7 – Number of main technical components of the supply chain designed.**

| Plant | AEC (1 MW) | AEC (5 MW) | AEC (10 MW) | AEC (50 MW) | Tube trailer | Pressure tank ($H_2$) | Pressure tank ($O_2$) |
|---|---|---|---|---|---|---|---|
| Scenario A | | | | | | | |
| #2 | 1 | | 3 | | 10 | 1 | 3 |
| #4 | 1 | 1 | 3 | 3 | 57 | 6 | 15 |
| #5 | 3 | | 2 | | 8 | 1 | 2 |
| #6 | 1 | 1 | 2 | 2 | 39 | 5 | 11 |
| AM | | | | | | 117 | |
| Scenario B | | | | | | | |
| #2 | 6 | 1 | 2 | | 10 | 1 | 3 |
| #4 | 11 | 5 | 15 | | 57 | 6 | 15 |
| #5 | 3 | | 2 | | 8 | 1 | 2 |
| #6 | 11 | 3 | 10 | | 39 | 5 | 11 |
| AM | | | | | | 117 | |
| Scenario C | | | | | | | |
| #2 | 1 | | 3 | | 10 | 1 | 3 |
| #4 | 11 | 1 | 7 | 2 | 57 | 6 | 15 |
| #5 | 3 | | 2 | | 8 | 1 | 2 |
| #6 | 11 | 1 | 6 | 1 | 39 | 5 | 11 |
| AM | | | | | | 117 | |
| Scenario D | | | | | | | |
| #2 | 1 | | 3 | | 10 | 1 | 3 |
| #4 | 11 | 1 | 7 | 2 | 57 | 6 | 15 |
| #5 | 3 | | 2 | | 8 | 1 | 2 |
| #6 | 11 | 1 | 6 | 1 | 39 | 5 | 11 |
| AM | | | | | | 117 | |

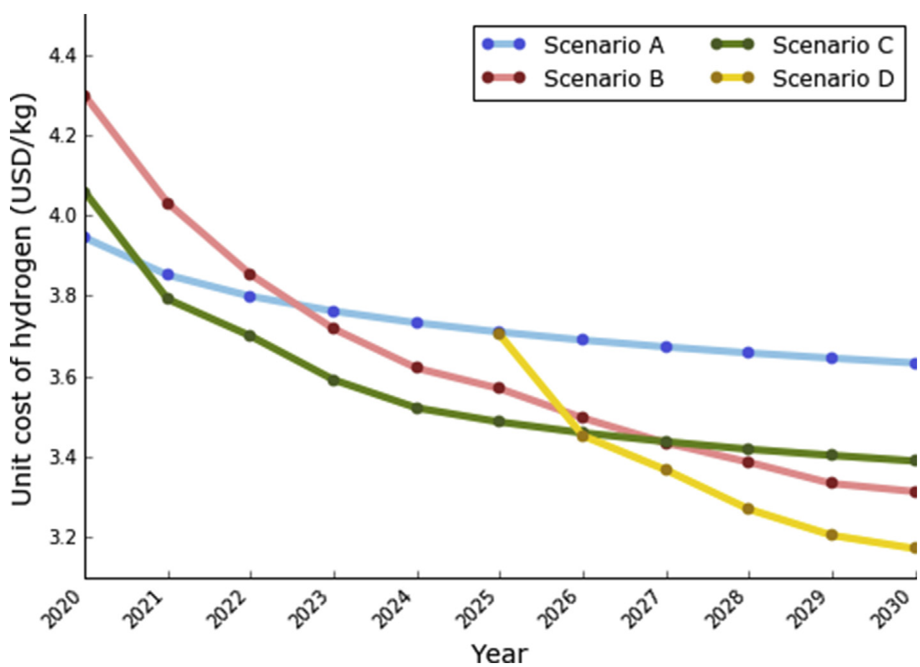


**Fig. 4 – Unit cost of green hydrogen from 2020 to 2030. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)**

production starts 5 years later in Scenario D, this scenario has the smallest total production volume – about 212.5 kt.

In contrast, however, the results regarding LCOHs illustrate exactly the opposite. Scenario D has the lowest LCOHs in both two cases (3.91 and 3.30 USD/kg respectively). LCOHs in Scenario B are almost the same with that of in Scenario C. Although hydrogen production volume is the largest in Scenario A, however, it has the highest LCOHs – 4.36 and 3.76 USD/kg respectively. Obviously, Scenario D is the most cost-effective of the four energy transition modes, indicating that decreases in electricity and facility prices are larger contributors to the future cost of hydrogen than cost advantages from economies of scale and technology learning effect through improving manufacturing processes. The study [79] also supports the view that cost reduction in renewable electricity and electrolysers will increase the use of green hydrogen and make it more competitive.

*Breakdown of the cost of hydrogen*. Additionally, in order to understand the proportion of each part, LCOHs are further decomposed into sections: production, transport, storage and oxygen sales (in those cases where oxygen is considered), which refers to the balance between income from oxygen sales and related infrastructure investment and operating expenses.

As shown in Fig. 6, LCOHs of two cases (with/without oxygen valued) are shown out on left and right side respectively. Obviously, production is the largest portion of the LCOH, and the share of each part does not see a distinct difference between scenarios for both cases. Additionally, a sensitivity analysis is carried out (in Section Model evaluation) that reveals the main contributors in the production section.

In the non-oxygen case, the production part contributes the most to the total LCOH, which is above 79 % in all scenarios, followed by the transport part, ranging from 12.0 to 12.6 %. The storage part is the least, constituting 7.8–8.1 % of the total share.

Besides, in the case where oxygen sales is considered, oxygen sales have the total LCOH reduced by 12.2–13.5 %. The share is even slightly higher than that of the transport part in most cases, which is around 10.5–10.9 % by scenarios. Production is still the largest proportion, which is above 68 % in all scenarios. The share of storage is still the least, ranging from 6.8 to 7.0 %. Hence, we come to a conclusion that with an oxygen price of 85 USD/t, selling by-product oxygen can basically offset green hydrogen cost in transport or storage.

*Levelized cost of ammonia*. The levelized cost of green ammonia (LCOA) in the next decade is also calculated to compare with the current production costs. In addition to the hydrogen produced by renewable energy, the green ammonia synthesis requires an air separation unit (ASU) to separate nitrogen from the air, and an energy input with hydrogen and nitrogen fed into a Haber-Bosch ammonia synthesis loop [80].

In the past decade, the price of ammonia produced from fossil fuels fluctuated between 2000 and 3500 CNY/t due to volatile raw material prices, and the average gross margin is 5 % [81,82]. We apply the average prices in the present ammonia industry [83]. Fig. 7 shows the contrast between fossil fuel-based and renewable-based ammonia production costs. The costs of green ammonia are calculated on the basis of the LCOHs in the four scenarios with oxygen-related expenses and incomes included and excluded respectively. In general, the production cost of green ammonia without oxygen being valued is 1.5–2 times higher than the present level indicating there is still a large cost difference between fossil fuel-based and renewable-based ammonia in the next decade. This is basically consistent with findings in some recent works estimating LCOAs in other countries (e.g. LCOAs estimated range from 7 to 800 USD/t in the work [84,85]), but even higher than those. This is mainly caused by the fact that other than only focusing on the production phase of green ammonia, the entire supply chain are examined in this study with hydrogen production, transport and storage in each renewable power plant taken into account. That also indicate, in addition to the production process, costs from other parts of the supply chain also have obvious effects to the overall costs and should not be neglected.

In addition, by-product oxygen presents evident economic benefits that LCOAs can be reduced to the level of being 1–1.5 times higher than the current production cost when oxygen is considered.

### Model evaluation

Model evaluation is a necessary process to ensure the appropriateness of the model and to examine the influence of

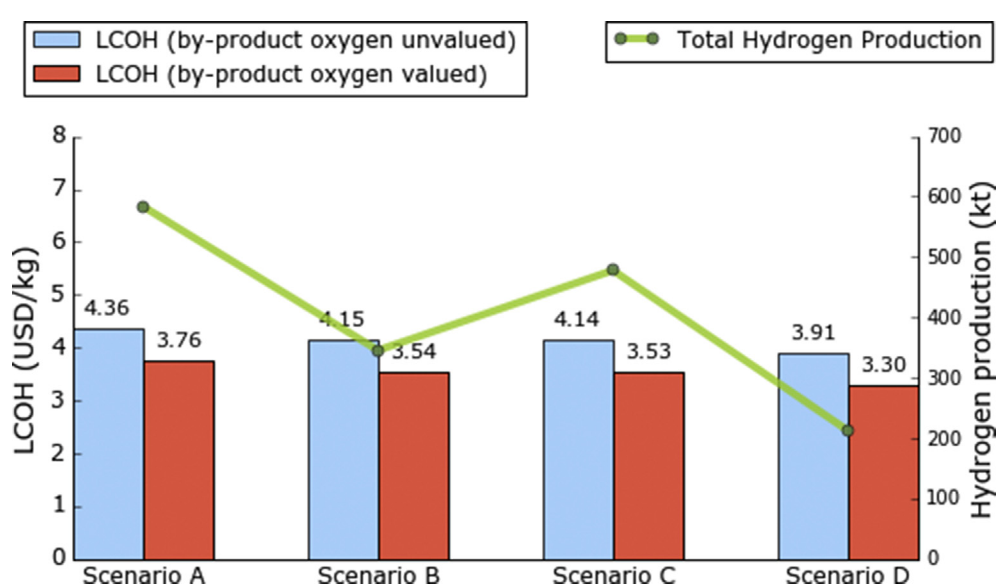


**Fig. 5 – LCOHs and green hydrogen production volumes. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)**

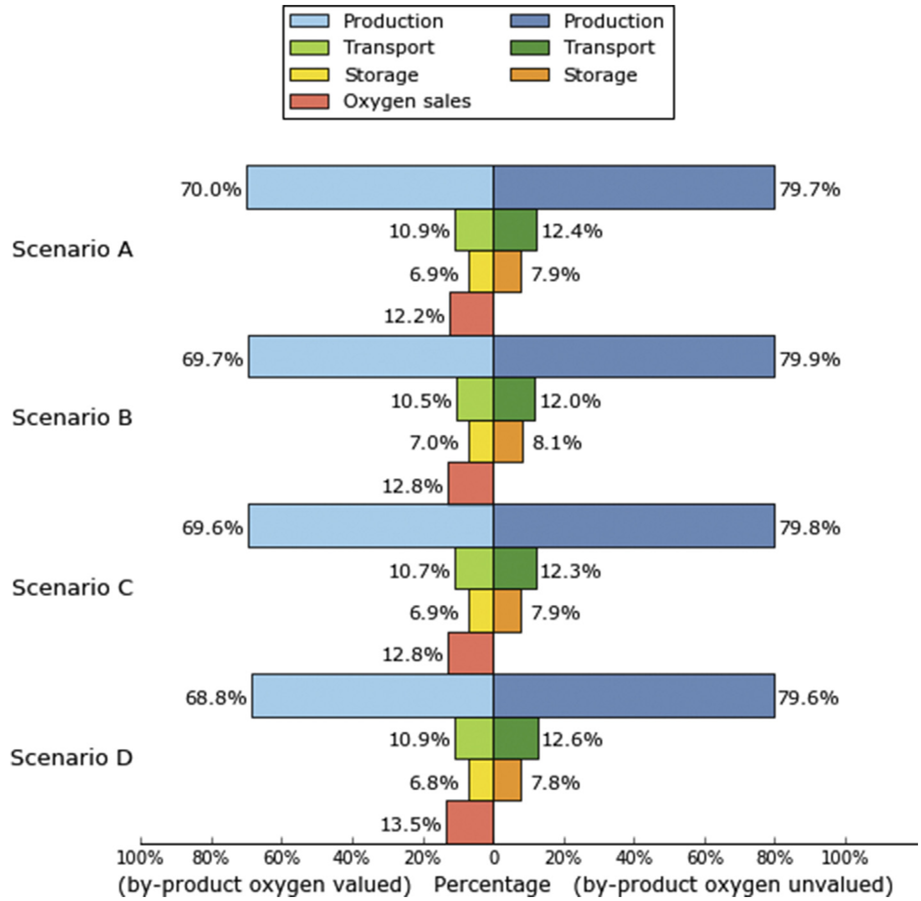


**Fig. 6 – Cost breakdown of green hydrogen. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)**

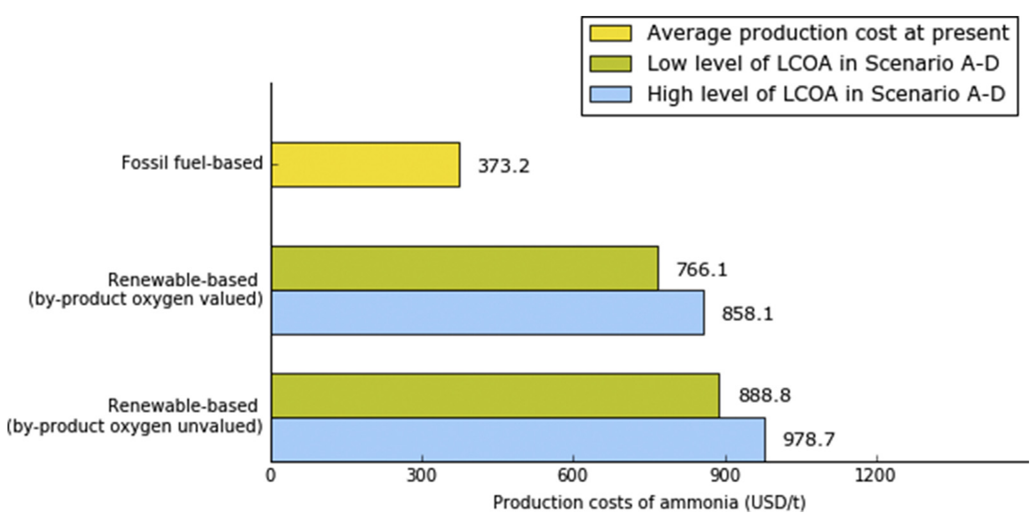


**Fig. 7 – Comparison between renewable-based and fossil fuel-based ammonia production costs.**

uncertainties on the results. We followed the behaviour tests recommended in the work [86].

First, an extreme condition test was conducted to check whether the outputs are logical when some of the inputs are set to extreme conditions. No renewable hydrogen and oxygen is produced when the annual growth rate of green hydrogen demand is set to zero. As mentioned above, Scenarios B, C and D have a multi-year time span in implementation of the new hydrogen supply system. The annual production costs in these three scenarios show less decreases if the expenses in procurement of facilities are not time-dependent in the next decade. These results from the model match well with actual behaviour under the same situations.

Second, sensitivity analysis was conducted to check the effects of uncertain parameters on the final results. A set of main parameters were examined on the basis of Scenario A and the results are shown in Table 8.

We found that the electrical efficiency of electrolysers and renewable electricity price have a substantial impact on driving down the green hydrogen cost. The overall cost can be reduced by 9.0 % if electrical efficiency is improved by 10 %, and a 20 % drop in electricity price induces a 13.8 % cost decline. Electrolyser price is also a sensitive factor, but less sensitive than the prior two. A 20 % price decrease in electrolysers brings the total cost down by 4.2 %, which is still much more significant than the price decreases in transport tools and storage tanks, due to the large share of production in the LCOH. The improvement in transport capacity contributes less to reducing the LCOH; a 15 % rise in transport capacity only brings down the total cost by 0.5 %. Additionally, we also examine the impact of the oxygen price on the LCOH. In the past a few years, the industrial oxygen price has been volatile in China, fluctuating between 400 and 1200 CNY/t (i.e. equivalent to 57–171 USD/t). Results show that LCOH can be reduced by 18.3 % when the oxygen price stays at 171 USD/t, and the share shrinks to 6.1 % when the price goes down to the lowest level. Hence, although the oxygen sales price is not a large contributor to the cost of hydrogen, it is however, expected that oxygen price can still exert a great impact on the LCOH as the price has varied greatly in the past.

## Discussions and policy implications

China's ammonia industry consumes considerable amounts of hydrogen each year. Hence, it is potentially a large market for green hydrogen application which will play an important role in future energy transition of China. Based on the results of this study, main findings are summarized as follows:

1) Wind power is a preferable energy source for power to hydrogen in China for the next decade, as it is more abundant and cheaper than other renewable energy sources, such as solar or biomass energy.
2) Although liquid storage can improve the energy density effectively, gaseous transport and storage remain the primary solutions in the next decade due to lower energy and investment costs required for compression than for liquefaction.
3) Production represents the largest proportion of the total cost of hydrogen. In the case study, we found it represents over 80 % share of total cost, however, transport as well as storage combined only contribute about 20 %. Selling by-product oxygen can be an effective way to offset the expenses of green hydrogen production. A cost reduction of about 10 % can be achieved by oxygen sales at a price of around 85 USD/t, which could basically cover the expenses of hydrogen transport or storage. We note, however, that price fluctuation in the oxygen market has been considerable in the past, which will represent a risk for the running of this business in the future as it places great uncertainty on the effectiveness of this offset. We stress that although these figures may change by pattern of supply chain and case study selected, findings obtained remain valid.
4) In the four scenarios, the cost of hydrogen can be reduced by 7–23 %, depending on the scenario. In addition, we found that starting the energy transition in the second half of next decade is the most cost-effective in all of the scenarios, with both the lowest hydrogen production volume and lowest LCOH (3.3 USD/kg). This indicates that decreases in electricity and facility prices contribute more to reducing the future cost of hydrogen than cost advantages from economies of scale and learning effect from improving manufacturing processes. The results of the sensitivity analysis also support this conclusion, where we found that electrical efficiency of electrolysers, electricity price and electrolyser price are the most significant driving factors influencing the LCOHs.
5) The green ammonia production cost is also estimated against potential LCOHs obtained for the next decade. We found that the production cost of green ammonia will be at least twice that of the present level.

As the case study is selected in the region of Inner Mongolia which owns the most abundant renewable energy resources, lowest renewable electricity prices and large-scale ammonia industry, the results may represent the most agreeable

**Table 8 – Results of the sensitivity analysis.**

| Test Item | LCOH (USD/kg) | Share of hydrogen production | Share of hydrogen transport | Share of hydrogen storage | Share of oxygen profit |
|---|---|---|---|---|---|
| Prices of electrolysers drop by 20 % | 3.59 | 68.9 % | 11.3 % | 7.2 % | 12.6 % |
| Electrical efficiency of electrolysers rises by 10 % | 3.43 | 67.9 % | 11.7 % | 7.4 % | 13.0 % |
| Electricity prices for electrolysis drop by 20 % | 3.23 | 66.5 % | 12.2 % | 7.7 % | 13.6 % |
| Capacities of transport tools rise by 15 % | 3.70 | 70.9 % | 9.8 % | 7.0 % | 12.3 % |
| Prices of transport tools drop by 20 % | 3.74 | 70.3 % | 10.5 % | 7.0 % | 12.2 % |
| Prices of hydrogen storage tanks drop by 20 % | 3.70 | 70.9 % | 11.0 % | 5.8 % | 12.3 % |
| Prices of oxygen storage tanks drop by 20 % | 3.74 | 69.8 % | 10.9% | 6.9 % | 12.4 % |
| Oxygen price drops to 57 USD/t | 3.98 | 73.3 % | 11.4 % | 7.3 % | 8.0 % |
| Oxygen price rises to 171 USD/t | 3.07 | 61.5 % | 9.6 % | 6.1 % | 22.8 % |

conditions in China for the next decade. As a result, policy implications are given as follows:

1) We suggest taking a moderate step forward in green ammonia production in the next decade, in order to avoid unnecessarily high social and governmental investment. This is because the price of green ammonia will still be much higher in the next decade due to the high production cost of green hydrogen. The decline of renewable electricity and infrastructure facility prices and the improvement in electrical efficiency of electrolysers, which are key drivers for bringing down the future green hydrogen cost, present opportunities.
2) More policies should be focused on reducing the electricity price and facility-related investments costs to bring down the LCOHs, for example enacting related subsidy mechanisms.
3) We stress the importance of sector integration to offset the high cost of green hydrogen production. In this paper, we show that by-product oxygen sales could partly offset the total expense of green hydrogen production, meanwhile providing high-quality oxygen for industrial and medical use. This is a promising potential integration of these two industry sectors. But it also should be noted that the volatile oxygen price might pose uncertainties and risks to the effectiveness of the offset.

Besides, our study has some limitations. First, the results obtained are based on average hourly hydrogen production volume, so the time period set for storage can be adjusted in the light of the actual conditions and costs will be further increased due to fluctuations in the hydrogen production capacity. Second, in this study we set each single expansion period as one year; it can also, however, be adjusted to a multi-year period, and it can differ with one another. Third, this study concerns one possible supply system design, and the results obtained from the case study cannot reflect all possible conditions in China. So strategies and feasibilities by region and by supply system can be further explored in a following study. However, this does not compromise the conclusions and implications of this study. It is because of the finding that production cost is dominant in terms of the total expense, which will not vary by supply system, and the case study selected represents the favourable conditions in China. Finally, more policy-related studies can be carried out by involving social interactions in the simulation process. This will also be improved and explored in the future work.

## Conclusions

This paper has explored supply chain design and expansion planning of green ammonia production in China in the next decade with a case study in the Inner Mongolia region. Given that traditional optimization approaches fail to capture the complexity and dynamics of an energy transition, a hybrid optimization-based simulation approach is developed. A number of uncertainties are considered, such as expansion speed, scale of the economy, learning effect, capital investments, renewable electricity prices, etc. In addition, oxygen as a by-product of green hydrogen production is also taken into account to evaluate its economic effects to the overall production costs. In the case study, we simulated the supply chain expansion by creating four scenarios representing different transition pathways. We found that production cost of green ammonia will be at least twice that of the current level due to hydrogen is produced based on a green supply chain. In addition, production accounts for the largest share of the overall expenses of green hydrogen. The decline of electricity and electrolyser prices are identified as the key factors in driving down the costs of green hydrogen. Selling by-product oxygen can be an effective way to offset the expenses of green hydrogen production, however, fluctuations in oxygen sales price may pose uncertainties to the effectiveness of the offset. As results obtained from the case study possibly represents the optimal conditions in China for the decades ahead due to the large scale of the ammonia industry and abundant renewable energy resources in this region, we propose to take a moderate step towards green ammonia production, and more policies should be focused on reducing the electricity price and capital investments in green hydrogen production. We assume the findings and policy implications obtained may shed light on strategies for future green ammonia production and energy transition in China. Besides, the approach we proposed can be used for reference in analysing other cases not unique to China.

## Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

## Acknowledgements

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## Nomenclature

*Abbreviations*

| | |
|---|---|
| AEC | Alkaline electrolyser |
| ASU | Air separation unit |
| CG | Coal gasification |
| CRF | Capital recovery factor |
| ESS | Expanded supply system |
| FCV | Fell cell vehicle |
| IOS | Iterative optimization-based simulation |
| LCA | Life cycle assessment |
| LCOA | Levelized cost of ammonia |
| LCOH | Levelized cost of hydrogen |

MILP Mixed integer linear programming
NG Natural gas
P2G Power to gas
PEMEC Proton exchange membrane electrolyser
SD System dynamics
SMR Steam reforming
SO Simulation-optimization
SWOT Strengths-weakness-opportunities-threats

*Datasets*

*HCR(n)* Economic information of the hydrogen supply system at the *n*th year, such as annual expense, hydrogen unit cost, cost breakdown, etc.
*HP(n)* Hydrogen production amount of the *n*th year
*HSD(n)* The design for hydrogen supply system expansion at the *n*th year, including the number and types of facility for production, transport and storage on power plants or the ammonia plant
*HSS(n)* The hydrogen supply system infrastructure at the *n*th year
*IC(n)* Capital investment expenses of unit hydrogen production, storage and distribution at the *n*th year
*PR(n)* The penetration rate of renewable hydrogen supply system of the *n*th year
*TEP(n)* Technical and economic parameters as inputs for optimization model, including facility prices, installed capacity for the *n*th year, and existing infrastructure and cost related information of the *n*-1 th year

*Indexes*

*a* Ammonia production site
*e* Type of electrolysers
*f* Power plant
*r* Type of oxygen storage tank
*s* Type of hydrogen storage tank
*t* Type of hydrogen transport tool

*Variables*

$HP_{n,f}$ Hydrogen production rate at the power plant *f* in the *n*th year-, kg/d
$O_{n,f,r}$ Oxygen inventory in storage tanks *r* at the power plant *f* in the *n*th year, kg
$O^{cost}{}_{n}$ Oxygen storage cost in the *n*th year, USD/yr
$O^{cost}{}_{n,f,r}$ Cost relating to all the oxygen storage tanks *r* at the power plant f in the nth year, USD
$ON_{n,f,r}$ Number of the oxygen storage tanks *r* required at the power plant *f* for the *n*th year, dimensionless
$O^{rev}{}_{n}$ Income of oxygen sales at the power plant *f* in the *n*th year, USD/yr
$OP_{n,f}$ Oxygen production rate at the power plant *f* in the *n*th year, kg/d
$P_{n,f,e}$ Capacity of all the electrolysers *e* on the power plant *f* in the *n*th year, KW
$P^{cost}{}_{n}$ Hydrogen production cost in the *n*th year, USD/yr
$P^{cost}{}_{n,f,e}$ Cost relating to all the electrolysers *e* at the power plant *f* in the *n*th year, USD/yr
$PN_{n,f,e}$ Number of the electrolysers *e* required at the power plant *f* in the *n*th year, dimensionless
$S_{n,a,s}$ Hydrogen inventory in storage tanks *s* at the ammonia plant in the *n*th year, kg
$S_{n,f,s}$ Hydrogen inventory in storage tanks *s* at the power plant *f* in the *n*th year, kg
$S^{cost}{}_{n}$ Hydrogen storage cost in the *n*th year, USD/yr
$S^{cost}{}_{n,a,s}$ Cost relating to all the storage tanks *s* at the ammonia plant in the *n*th year, USD/yr
$S^{cost}{}_{n,f,s}$ Cost of all the hydrogen storage tanks s at the power plant *f* in the *n*th year, USD/yr
$SN_{n,a,s}$ Number of the hydrogen storage tanks *s* required at the ammonia production plant in the *n*th year, dimensionless
$SN_{n,f,s}$ Number of the hydrogen storage tanks *s* required at the power plant *f* in the *n*th year, dimensionless
$T_{n,f,t}$ Hydrogen distribution rate by transport tools *t* required at the power plant *f* in the *n*th year, kg/d/round
$T^{cost}{}_{n}$ Hydrogen distribution cost in the *n*th year, USD/yr
$T^{cost}{}_{n,f,t}$ Cost relating to all the transport tools *t* in the *n*th year, USD/yr
$TN_{n,f,t}$ Number of the transport trucks *t* required at the power plant *f* in the *n*th year, dimensionless
* All the variables are subject to the ESS of each year

*Parameters*

$CF^{ho}$ Coefficient for calculation of oxygen production rate with hydrogen production rate, dimensionless
$CF^{hp}{}_{e}$ Coefficient for calculation of hydrogen production rate with the capacity of electrolysers *e*, dimensionless
$D_f$ Distance from the power plant *f* to the ammonia plant, km
*dr* Discount rate, dimensionless
$E^{prc}{}_{n}$ The price of electricity for hydrogen production in the *n*th year, USD/KWh
$HD_n$ The incremental daily green hydrogen demand in the *n*th year, kg/d
*m* Lifetime of a project or facility, yr
$HP^{max}{}_{f}$ Maximum hydrogen production rate at the power plant *f*, kg/d
$O_r^{cap}$ Unit capacity of oxygen storage tanks *r*, kg
$O^{crf}{}_{r}$ Capital recovery factor of storage tanks *r*, dimensionless
$O^{invcost}{}_{n,r}$ Unit investment cost of oxygen storage tanks *r* in the *n*th year, USD/kg
$O^{optcost}{}_{n,r}$ Annual unit operating cost of oxygen storage tanks *r* in the *n*th year, USD/kg/yr
$O^{mcost}{}_{n,f,r}$ Miscellaneous expenses for the *r*th type of oxygen storage at the power plant *f* in the *n*th year, including installation expense, and expenses of other facility, etc., USD/yr
$O^{prc}$ Oxygen price, USD/kg
$P^{cap}{}_{e}$ Unit capacity of electrolysers *e*, KW
$P^{crf}{}_{e}$ Capital recovery factor of electrolysers *e*, dimensionless
$P^{invcost}{}_{n,e}$ Unit investment cost of electrolysers *e* in the *n*th year, USD/KW
$P^{optcost}{}_{n,e}$ Annual unit operating cost of electrolysers *e* in the *n*th year, USD/KW/yr
$P^{mcost}{}_{n,f,e}$ Miscellaneous expenses of the *e*th type of hydrogen production at power plant *f* in the *n*th year, including expenses of construction and installation, etc., USD/yr

$S^{cap}{}_{s}$ Unit capacity of hydrogen storage tanks s, kg
$S^{crf}{}_{s}$ Capital recovery factor of storage tanks s, dimensionless
$S^{hsp}{}_{a}$ The given time period of hydrogen storage at the ammonia plant, d
$S^{invcost}{}_{n,s}$ Unit investment cost of hydrogen storage tanks s in the *n*th year, USD/kg
$S^{optcost}{}_{n,s}$ Annual unit operating cost of hydrogen storage tanks s on the power plant *f*, USD/KW/yr
$S^{mcost}{}_{n,a,s}$ Miscellaneous expenses of the *s*th type of hydrogen storage at the ammonia plant in the *n*th year, including expenses of construction and other facility, etc., USD/yr
$S^{mcost}{}_{n,f,s}$ Miscellaneous expenses of the *s*th type of hydrogen storage at the power plant *f* in the *n*th year, including expenses of construction and other facility, etc., USD/yr
$S^{osp}{}_{a}$ The given time period of oxygen storage at the power plant *f*, d
$SP_a$ The given time period of hydrogen storage on the ammonia plant, d
$T^{cap}{}_{t}$ Unit transport capacity of transport tools t, kg
$T^{crf}{}_{t}$ Capital recovery factor of transport tools *t*, dimensionless
$T^{dts}{}_{n,f,t}$ Transport distance of transport tools *t* for the power plant *f* in the *n*th year, km/yr
$T^{invcost}{}_{n,t}$ Unit investment cost of hydrogen transport tools *t* in the *n*th year, USD/kg
$T^{optcost}{}_{n,t}$ Annual unit operating cost of transport tools *t* in the *n*th year, USD/kg/yr
$T^{fcost}$ Fuel cost for hydrogen transportation, USD/km
$T^{feq}{}_{f,t}$ Transport frequency of transport tools *t* at the power plant *f*, round/d
*WH* Annual operating hours, h
*WD* Annual operating days, d

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