

Techno-economics of ammonia as an energy carrier. Exporting wind from the North Atlantic Ocean/North Sea to Wales

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Abstract

The United Kingdom (UK) has already established several goals for producing hydrogen from offshore wind energy resources. However, how to transport this energy is still not known. Based on this context, this work was aimed at analyzing ammonia as an energy carrier that could help the UK to exploit and move these resources by quantifying its techno-economics. The objective of this work was also to analyze this case by only considering hydrogen as the energy carrier. Six scenarios were studied and the results show that the alternative with the lowest levelized cost of hydrogen (LCOH) was the use of ammonia as the energy carrier from Orkney (Scotland) to the Milford Haven Port (Wales) via maritime transportation and its decomposition back to hydrogen without its purification. The LCOH for this scenario was 9.93 USD per kg of H₂, which was 0.93 USD per kg of H₂ and 2.53 USD per kg of H₂ lower in comparison to directly transporting liquid hydrogen or considering the purification of hydrogen via ammonia, respectively. The construction of a hydrogen pipeline from Orkney (Flotta Oil Terminal) to the Milford Haven Port was the next best alternative (11.23 USD per kg of H₂), while transporting hydrogen or ammonia via the Teesside Free Port (England) with maritime carrier and pipeline were the highest cost alternatives. A sensitivity analysis was carried out considering different levels of grid electricity and offshore wind costs highlighting an important impact of the first particularly on hydrogen production costs. As a conclusion, we show that ammonia is a feasible energy carrier that represents a large-scale solution comparable to hydrogen in terms of costs that has the advantage of a relatively rapid deployment while hydrogen (particularly its transport and storage) reaches a more mature stage of development.

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Introduction

The reduction of greenhouse gas (GHG) emissions requires the deployment of a large portfolio of alternatives. While the electrification of activities based on renewable sources represents the main option for accomplishing the latter, the use of energy vectors such as hydrogen or ammonia will also play an important role to further reduce emissions in different sectors of the economy. In recent years, there has been an increasing interest in green hydrogen and there have been important efforts to develop its supply chain as soon as possible. While research has focused on understanding the production of green hydrogen; its storage, transport and distribution still needs to be further studied [1]. These latter elements of the supply chain entail several difficulties for hydrogen and because of this, other chemical compounds have been proposed to serve as hydrogen carriers [2]. Ammonia corresponds to one of these alternatives, being

attractive because of its low-cost and extended use in several sectors.

The work here presented has aimed at analyzing in detail the techno-economics of green ammonia's supply chain as an alternative to harness offshore wind energy from the North Atlantic Ocean/North Sea [3]. As stated by [4-5], Scotland has abundant renewable resources (particularly wind) which could be used for green hydrogen production. The Scottish government has analyzed the potential and costs for producing this energy vector. While this initial work has shown the feasibility of producing green hydrogen, its storage, transport, distribution, and use remains unknown. The techno-economic analysis presented here focuses on the large-scale transportation of green ammonia and hydrogen to the port of Milford Haven in Wales (Fig. 1). It is important to mention that while ammonia has been studied as a hydrogen carrier in several studies and compared to other hydrogen carriers [1, 2, 6], this work integrates a complete supply chain from

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hydrogen to hydrogen via ammonia. In addition, this work provides a detailed engineering cost analysis of ammonia decomposition complementing existing studies [7-10].

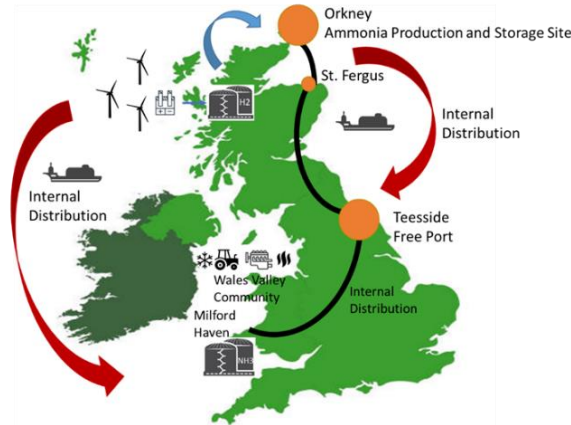


Fig. 1. Transportation routes of green ammonia and hydrogen (taken and modified from [11]).

Materials and Methods

In this work, Aspen Hysys Version 12 was used to design the ammonia Haber-Bosch process, the Air Separation Unit (ASU), the ammonia storage, pipeline transport systems, and the ammonia cracking plant. Additionally, a hydrogen liquefaction plant was also designed. The technical analysis was based on several sources of information in the literature which will be presented in detail later. At this point of the research, liquefied hydrogen was considered as the main energy transport mode because of its similarity with the liquefied natural gas (LNG) supply chain and because of current developments. However, compressed hydrogen transport was also considered because of recent announced plans to create a hydrogen transmission backbone in the United Kingdom (UK) [12]. The engineering design and economic analysis were used to calculate the levelized cost of hydrogen (LCOH) and the economic performance of six scenarios was assessed. The production of hydrogen was evaluated in a simplified manner together with the production of offshore wind energy considering the wind characteristics of a specific point in the North Atlantic Ocean/North Sea. The scenarios describe various alternatives for hydrogen delivery at Milford Haven. The selection of the specific locations was based on existing government plans or announcements for hydrogen development in the UK.

- Scenario A. Hydrogen production from wind energy in Orkney and its use for ammonia production via the Haber-Bosch process considering an ASU and storage. Maritime transportation from Orkney to the Milford

Haven Port and its storage and decomposition to hydrogen via thermal cracking.

- Scenario B. Ammonia production as in Scenario A, but maritime transportation from Orkney to the Teesside Free Port and its storage and transportation via pipeline to the Milford Haven Port with its storage and decomposition to hydrogen via thermal cracking.
- Scenario C. Hydrogen production from wind energy in Orkney and its liquefaction, storage, and maritime transport to the Milford Haven Port (storage and regasification was also considered).
- Scenario D. Hydrogen production as in Scenario C, but maritime transport to Teesside and pipeline transport to the Milford Haven Port (storage and regasification were also considered).
- Scenario E. As Scenario A, but the ammonia cracking unit does not consider hydrogen purification.
- Scenario F. Hydrogen transport via offshore and onshore pipelines from Orkney to Milford Haven through the St. Fergus Gas Terminal and the Teesside Free Port.

With regards to the economic analysis, bare module cost (C_{BM}) analysis was used for most of the processes using the following equation for each scenario and process equipment (i), where K_1 , K_2 and K_3 (values presented in Table 1A in the Annex) are constants and A corresponds to their capacity [13, 14].

$$\log_{10} C_{BMi} = K_1 + K_2 \log_{10} A + K_3 (\log_{10} A)^2 \quad (1)$$

The estimated costs are in USD of 2001 and for this reason, they were adjusted to 2022 prices with the use of the Chemical Engineering Price Cost Index (CEPCI) [15]. The estimated bare module costs were also adjusted considering the process pressure and required equipment materials which in most cases was stainless steel and carbon steel [13, 14]. For some of the process equipment, the limits of application of the capital cost equation were surpassed and, in these cases, costs were adjusted considering the following equation.

$$C_1 = C_2 \left(\frac{S_1}{S_2} \right)^\alpha \quad (2)$$

In this equation, C_1 represents the cost for the new equipment capacity (S_1) while C_2 the cost for the existing capacity (S_2). The constant α (with a value of 0.6) considers the economies of scale and the increasing returns to scale which commonly applies to process equipment [16]. For some of the parts of the process, costs were not estimated using this

procedure and information from the existing literature was reviewed. Exchange rates were taken from the Bank of England to adjust these costs from different currencies [17].

The fixed capital investment of a process plant (*FCI*) is comprised by direct plant costs (*PPC*) and indirect plant costs (*IPC*) [18]. The Lang factor technique for total capital costs uses several factors that adjust equipment costs and help calculating the *PPC* and *IPC* of a process plant [14, 18]. The *PPC* was calculated using the following equation [19]:

$$PPC = (1 + f_1 + f_2 + f_3 + f_4 + f_5) \sum_{i=1}^n C_{BM_i} \quad (3)$$

For this work, only the values for equipment erection (f_1), piping (f_2), instrumentation (f_3), electrical (f_4) and buildings and process (f_5) were considered. The value for the sum of the factors is 2.55. Finally, to obtain the *IPC*, the *PPC* was multiplied by a factor of 1.45, which includes design and engineering (f_{10}), contractor's fees (f_{11}), and contingency (f_{12}) [19].

$$IPC = (1 + f_{10} + f_{11} + f_{12}) \sum_{i=1}^n C_{BM_i} \quad (4)$$

The capital costs (*CAPEX*) were estimated by considering a working capital (*WC*) of 15% *FCI* with the following equation [19].

$$CAPEX = FCI + WC \quad (5)$$

The operating costs (*OPEX*) include variable (*VC*) and fixed costs (*FC*). For *VC*, electricity and catalyst costs were included in the estimation of *OPEX*. For this work, water costs were not included because of its marginal contribution to total costs [7]. In the case of electricity costs, they were taken as an average of 2022 electricity tariffs for non-domestic users presented by the Department of Energy Security and Net Zero (DESNZ) [20]. In the case of the facilities in Orkney, the levelized cost of electricity of offshore wind was used as input together with the previously mentioned electricity costs. The cost of the iron-based catalyst for the ammonia synthesis loop was taken from [21] and is equal to 0.21 USD per kg. For the ruthenium-based catalyst the cost was taken from [7] and corresponds to 37.5 USD per kg. Catalyst prices were adjusted using the US Consumer Price Index [22]. Fixed costs (*FC*) included the operating labour costs which were estimated using the following equation [13, 18],

$$Operators = (6.29 + 31.7P^2 \cdot 0.23NP) \cdot 0.5 \quad (6)$$

The previous equation estimates the number of operators per shift, and *P* represents the number of

particulate process stages while *NP* is the number of non-particulate process stages. As in [13], 4.5 operators per working operator (from equation 10) were considered. The operator salaries were taken from [23] and corresponds to the annual salary of an engineering technician (£35,988 per year). In addition to this, fixed costs incorporated maintenance (5.0% of *FCI*), laboratory costs (21.5% of operating labour), supervision (20.0% of operating labour), plant overheads (50.0% of operating labour), capital charges (10.0% of *FCI*) and insurance (1.0% of *CAPEX*) [18, 19]. It must be mentioned that all prices in this work were adjusted to 2022 values.

Results

Engineering analysis of hydrogen production, storage, and transportation routes

Offshore wind and hydrogen production

The interest in using offshore wind energy in Scotland has been moving forward and has been accelerating in the past few years. For instance, installed capacity for offshore wind in Scotland was 964 MW in 2021, increasing to 2,166 MW in 2022 [24]. For this work, offshore wind energy was determined to produce hydrogen and the selection of a potential site was based on existing government plans. The N1 option defined in the Sectoral Marine Plan for Offshore Wind Energy by the Scottish Government [25] was studied and the offshore wind farm calculations considered wind characteristics for this site. The N1 option has a total area of 1,163 m² and a potential for installing up to 2 GW [25]. As in [26], historical wind data was taken for this site, from the European Centre for Medium-Range Weather Forecasts Reanalysis v5 (ERA5) [27]. The calculation procedure and wind turbine data were taken from the work of [26]. The wind turbine power curve corresponds to a 10 MW DTU turbine with a cut-in speed of 4 m/s, a rated velocity of 11.4 m/s and a cutout velocity of 25 m/s. The turbine has a blade diameter of 178 m and a hub height of 119 m and has been used as reference in other studies [26]. Wind data from 1980 to 2022 was analyzed and capacity factors were calculated for a specific point with longitude -4.0 and latitude 58.8. For 2022, the estimated capacity factor was 0.57. The calculations did not consider any specific layout for the wind farm. The size of the wind farm was determined based on the electrolyzer requirements. It is important to mention that a large-scale system is considered, and back-up power might be needed to cope with the intermittency of offshore wind production. While batteries or high-pressure hydrogen storage could be an alternative, for simplicity, and because of the size of the system, electricity from the grid was assumed to power

electrolyzer when wind is not blowing. However, GHG emissions are associated with electricity consumption from the grid, thus, to have a fully decarbonized system, the first two options or low-carbon baseload generation alternatives must be considered in the future.

The Flotta Oil Terminal located in Orkney has been considered to become a hydrogen hub and there are plans to transform this terminal [28]. For this reason, as mentioned previously, hydrogen and ammonia facilities were assumed to be installed in this terminal and a HVDC subsea cable was considered to connect the offshore wind farm and the Flotta Oil Terminal. The approximate distance between these two points is 60 km and a 0.3% electrical loss per 100 km was also considered [29]. In the case of hydrogen production, a proton exchange membrane (PEM) electrolyzer was analyzed, and the design used the work of [29-31]. PEM electrolyzer can be stacked without losing efficiency or outlet pressure [29]. Because of this, 10 MW PEM electrolyzer units were included in the calculations. The hydrogen production facilities have a water desalination unit and compressors for the ammonia production system and its transport as a gas to St. Fergus. It is important to highlight that hydrogen leaves the electrolyzer at 60 °C and 30 bars [30]. Table 1 summarizes the main characteristics of these systems. For the ammonia production system, it was also considered that 312 tons per day of hydrogen could be delivered after its thermal cracking.

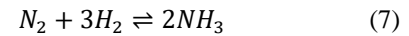
Table 1. Offshore wind electricity and hydrogen production systems.

System	Ammonia production	Liquid hydrogen	Gaseous hydrogen
Hydrogen produced (tons per day)	425	312	312
Number of electrolyzers	93	69	69
Water requirement (m ³ /h)	239	176	176
Offshore wind installed capacity (GW)	1.019	0.933	0.69
Generated power by the offshore wind system (GWh per year)	5,116	4,684	3,462
Electricity from the grid (GWh per year)	3,813	3,491	2,581

Ammonia route

Production at Orkney

Ammonia production was based on the Haber-Bosch process, in which H₂ and N₂ react in a catalytic reactor. It must be noted that the specific design of the ammonia production process is unique to every plant, but our design follows the general process and was revised considering the existing literature that particularly focuses on real large-scale systems taking several elements from references [13, 18, 32-39] that go from typical reactor pressures to general process configurations. For this work, heat integration calculations were not conducted [40]. For the ammonia synthesis loop, typical conditions were assumed for the process, mixing H₂ and N₂ in a 3 to 1 ratio, at a temperature of 400 °C and 200 bars. The chemical reactor for the synthesis loop was designed considering the following chemical reaction.



In this case a three-bed catalytic reactor is described by the reaction kinetics proposed by Temkin and Pyzhev [41, 42] with the following reaction rate equation.

$$r_{N_2} = \frac{f}{\rho_{Cat}} \left(k_1 e^{\frac{-87,090}{RT}} \frac{p_{N_2} p_{H_2}^{1.5}}{p_{NH_3}} - k_2 e^{\frac{-198,464}{RT}} \frac{p_{NH_3}}{p_{H_2}^{1.5}} \right) \quad (8)$$

In this equation r_{N_2} is the rate of reaction for nitrogen, p_i correspond to the partial pressures of every compound i (N₂, NH₃ and H₂) in bar, and f to a correction factor (value of 4.75) presented by [43, 44]. The pre-exponential factors k_1 (1.79x10⁴) and k_2 (2.57x10¹⁶) correspond to the forward and reverse reactions [44]. The reactor and the entire system were designed to produce 2,200 tons of ammonia per day. The ammonia synthesis reactor considers the recovery of heat between the first bed and the outlet, in addition to the extraction of heat between the second and third beds. The design was also confirmed by analyzing chemical equilibrium conditions [44]. For this design, the outlet stream from the synthesis loop has an NH₃ mole fraction of 0.167. The estimated total volume for the reactor was 37 m³ with a diameter of 2 m and a length of 11.8 m. For this reactor a bed void fraction of 0.5, a catalyst particle diameter of 0.006 m and a bulk density (ρ_{Cat}) of 2,650 kg per m³ were considered [45]. The pressure drop in each bed was calculated using Ergun equation for a packed column.

The products from the third bed of the reactor are cooled in a series of steps so that ammonia is condensed. In the condensation process, gases are separated and recycled back into the ammonia synthesis loop where they are combined with makeup reactants. This recycle stream is also used

to cool the products from the reactor. A small part of the gases in the condensation part of the process are eliminated and used for heat generation. Together with the condensation section of the process, a refrigeration cycle is included. Pressure is also

reduced to atmospheric conditions producing ammonia at $-33\text{ }^{\circ}\text{C}$. The following process diagram presents the design of the ammonia production plant (Fig. 2).

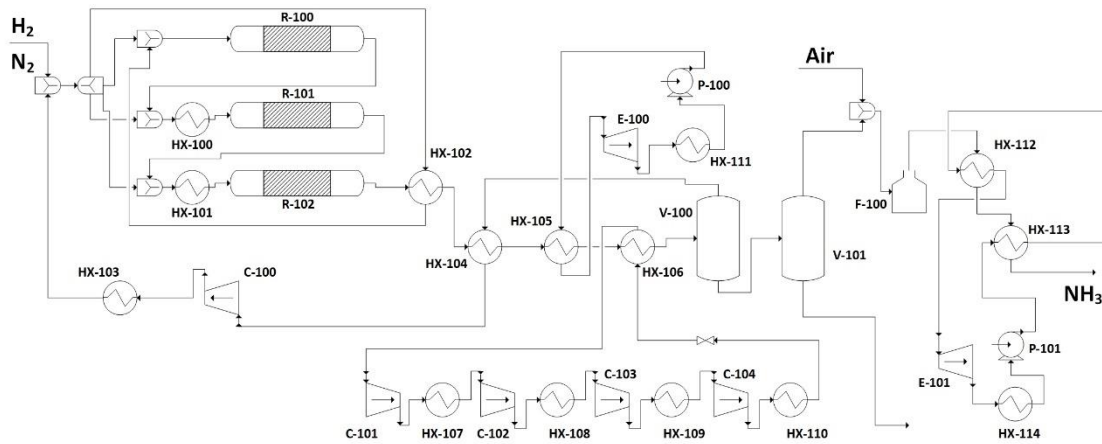


Fig 2. Ammonia production plant process diagram (see Nomenclature section).

The design of the ammonia plant included an air separation unit (ASU) to produce N_2 that is used in the synthesis loop. In this case, a cryogenic process was chosen because as highlighted by [13] the use of membrane separation or pressure swing adsorption is not realistically or economically feasible for large-scale production. The ASU was modelled based on a typical design to produce 2,946 kmole per hour. Figure 3 presents the ASU process diagram.

As part of the ammonia production facility, a storage system was also included. The storage of ammonia is commonly done with refrigerated tanks using insulated double containment tanks. The design of these tanks generally considers a storage time of 30 days which is based on the requirements of a typical chemical plant [13, 50, 51]. The storage facilities would require a tank with a capacity of 72,600 tons of ammonia (equivalent to $106,406\text{ m}^3$) considering a 10% additional freeboard [13]. The storage tank would 56.5 m wide and 42.4 m high. The distance between the inner and the outer tanks was considered as 1.5 m, and the total width would be 59.5 m. As highlighted by [52], there are storage facilities with this capacity for refrigerated ammonia tanks and the estimated dimensions are similar to those proposed. The refrigeration loop was also designed, and in this process, the boil-off is compressed and refrigerated following the design presented by [13] and [14, 50-54].

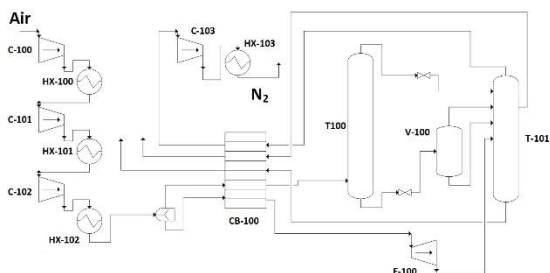


Fig 3. ASU process diagram (see Nomenclature section).

In the ASU, the difference in boiling points between N_2 , oxygen (O_2) and Argon (Ar) is used to separate them. The design was based on the work of [13, 46, 47] in which air is compressed, cooled, and purified and separated in multiple distillation columns. The produced nitrogen has a temperature of $-193.6\text{ }^{\circ}\text{C}$ and a pressure of 1.3 bar. This N_2 stream is later heated and compressed for the ammonia synthesis plant. For our work, an argon separation unit was not included [48, 49].

Maritime transport from Orkney to Teesside, pipeline transport to Milford Haven and storage

In this case, the transport of ammonia from the Orkney Ammonia Production and Storage Site to the Teesside Free Port was analyzed. For this purpose, and as highlighted by [55], the most common way of transporting ammonia for short distances corresponds to Medium Gas Carriers (MGCs) because of their lower costs. To perform this analysis the calculation of transport costs was based on the work of [51], [54] and [55]. Typical MGC characteristics (presented in Table 2) were assumed to estimate the number of required voyages to transport ammonia to the Teesside Free Port. The use of different sources of information was

minimized to have consistency with the calculations since not all the required data was available from the same source. It was also assumed that the potential MGC could use ammonia as fuel for propulsion since it is expected that ammonia fueled MGCs can be used commercially in the following years [56-58].

Table 2. Medium gas carrier (MGC) input data.

Gas carrier	MGC
Capacity (m ³) [55]	34,000
Speed of the vessel (loaded) (nm/hr) [55]	15
Loading rate (m ³ /hr) [55]	2,660
Propulsion power at nominal cruise speed (MW) [59]	9.5
Power for loading and unloading (MW) [50]	2.0

The calculation procedure followed the work of [56] and was based on estimating the total number of roundtrip voyages required per year to transport the produced ammonia at Orkney in addition to the total days required for the voyages. This information was used to calculate total costs. Initially, the required voyage time was estimated using the distance between ports (561.1 km) and obtained from [60]. Additionally, loading and unloading times were considered and to simplify calculations, it was assumed that they were the same. It must be noted that, these times are different since the unloaded amount of ammonia is smaller because of its use as a fuel for the MGC and the 4% capacity of the remaining heel at the demand point [51]. With this regard, the loaded amount of ammonia considered a usable capacity of 94% of total capacity [51]. The roundtrip time was estimated at 65.5 hours. The consumption of ammonia in an engine for propulsion purposes was also estimated considering an efficiency of 35%. Per voyage, 134 tons of ammonia are required for propulsion. The transport of ammonia would require 35 round trips with a total time of 96 days.

In the case of port storage, there is an interaction between charter costs and the size of storage that needs to be optimized following seasonal patterns and supply and demand [51]. For instance, [51] considered 1.7 weeks of storage in the demand port. In this case, if an average between these figures is considered (20 days), the storage facilities (Teesside and Milford Haven) would require a storage tank with a capacity of 48,400 tons of ammonia (equivalent to almost 71,000 m³) considering a 10% additional freeboard [13]. The storage tank would be 49.4 m wide and 37.0 m high, and the total width would be 52.4 m. In this case, the recovered boil-off

is equal to 9.28 tons per day which corresponds to 0.02% of the total storage. The total capacity of the compressors is 51.1 kW and the condenser duty is 181 kW.

The transport of ammonia via pipeline is common practice around the globe and only in the United States ammonia pipelines extend over 3,000 km and transporting almost 3 million tons per year [55]. The total pipeline length from Teesside to Milford Haven was calculated using the information of the existing natural gas network in the United Kingdom and following a pathway that goes through Leeds, Peterborough and Tirley [61]. The estimated distance was 809 km and considers route deviations [51]. From Tirley to the Milford Haven Port, the distance from the existing pipeline to Milford Haven was considered (316 km) [62]. For this work, an 18-inch diameter pipeline was contemplated together with pumping stations every 100 km with a pressure of 20 bars. The total duty of the pumps was estimated at 668 kW.

Maritime transport from Orkney to Milford Haven and storage

The direct maritime transport of ammonia from Orkney was also estimated and was based on the procedure presented before and based on the number of roundtrip voyages per year and the required days for the voyages. For this case, the distance between ports is 1,174.2 km [60]. The calculation of the roundtrip time used the same assumptions as for the transport to the Teesside Free Port. The roundtrip time corresponded to 110 hours because of the larger travelled distance in comparison to the Teesside case. The ammonia consumption for the ship engine was estimated at 249 tons per trip and the transport of ammonia requires a total time of 160 days.

Ammonia decomposition

Ammonia stored in Milford Haven can follow several routes according to its uses. For instance, it can be transported and used as a fertilizer, or combusted for electricity generation. However, ammonia can also be decomposed and converted into H₂ and N₂ through thermal cracking using a catalyst [10]. In this work, and to have a cost comparison of the different H₂ routes, full NH₃ conversion at Milford Haven was considered. The ammonia cracking system is based on the work of [7-10] and the process is presented in Figure 4.

For a large-scale system, the ammonia cracker follows a similar design to a steam methane reformer. In this process, the chemical reaction takes place within a firebox. In a typical reformer configuration, there is also a convection section for heat recovery and a furnace for flue gases. While the

design involves the use of several hundred tubes, the ammonia cracker in this work was modelled as a simple plug flow reactor. The design involved the production of up to 312 tons per day of hydrogen which is equivalent to the hydrogen quantities proposed for the hydrogen route from Orkney. In

this process, liquid ammonia from the storage tank is pressurized to 1.2 bars and vaporized, entering the cracker. In the reactor, the following chemical reaction occurs.

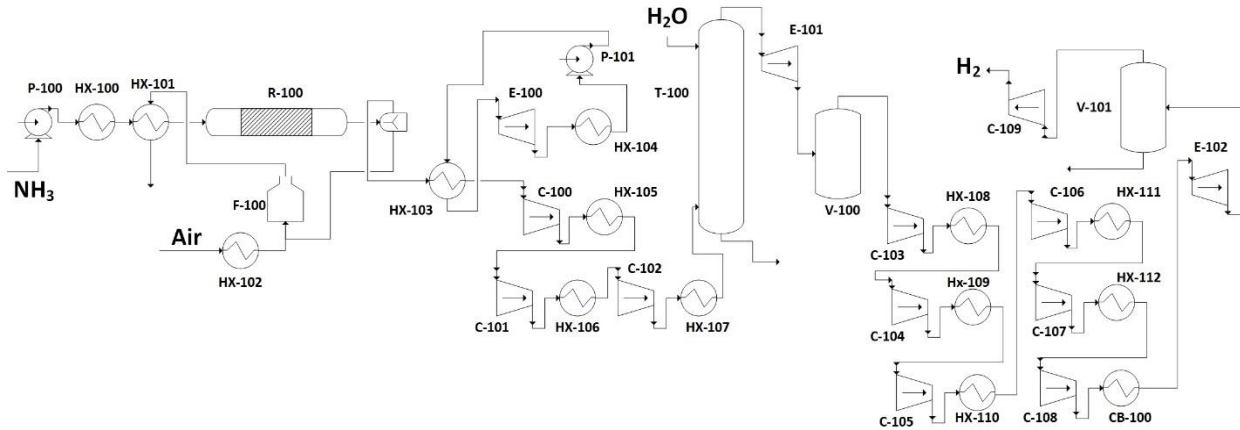
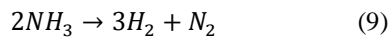


Fig. 4. Ammonia cracking system (see Nomenclature section).



For the ammonia decomposition, the Temkin and Pyzhev equation adequately describes the reaction kinetics with a Ruthenium catalyst at moderate temperature and pressure conditions [7].

$$-r_{NH_3} = k_3 e^{\frac{-117,000}{RT}} \left(\frac{p_{NH_3}^2}{p_{H_2}^3} \right)^\beta \quad (10)$$

In this equation r_{NH_3} is the rate of reaction for ammonia, and p_i correspond to the partial pressures of every compound i (NH_3 and H_2). The pre-exponential factor k_3 (1.19×10^8) and the reaction coefficient β (0.5) were taken from the work of [7, 63, 64]. The fire box design was simplified because of the lack of further information regarding its specific configuration and for this reason, individual tubes were not considered as in the work of [7]. However, the total length and diameter of the system is similar to the previously mentioned reference. The estimated total volume for the reactor was $2,500 \text{ m}^3$ with a diameter of 14.1 m and a length of 16.0 m. For this reactor a bed void fraction of 0.4, a catalyst particle diameter of 0.006 m and a bulk density of 588.0 kg per m^3 were considered [63, 64]. The pressure drop was also considered. The ammonia cracker is operated at a high temperature ($540 \text{ }^\circ\text{C}$) and low pressure, to maximize conversion which is above 99%. In this work, 19.5% of the reactor product is returned to the reactor furnace providing the energy for the chemical reaction [10]. The rest of the gas that leaves the ammonia cracker is cooled (a Rankine cycle is attached to this cooling step) and

enters a purification process that removes the unconverted NH_3 and N_2 and produces H_2 with a 99.99% purity. This section of the process follows the work of [7] and [8] and is initially based on the absorption of NH_3 with water in a column. The absorption column operates at 5 bar and its gaseous product is expanded to separate any water traces in a flash tank. The stream leaving this process enters a cryogenic cycle to remove N_2 . The stream is compressed to 240 bars and its temperature is reduced to $-195 \text{ }^\circ\text{C}$ in a cold box. The refrigerated stream is expanded and H_2 is separated in a flash tank. The product leaves the flash tank at $-233 \text{ }^\circ\text{C}$. The products from the flash tank (vapor and liquid) are used to reduce the temperature of the gases leaving the compression stage and the purified H_2 leaves the process at $15 \text{ }^\circ\text{C}$.

Hydrogen route

Liquefaction at Orkney and storage

The other route for transporting renewable energy to Milford Haven involves the direct use of hydrogen. In this case, a liquefaction process was designed for Orkney using existing designs developed by [65] and [66] and adjusted to produce 312 tons per day of liquid hydrogen. As in [65], to simplify the design, the ortho-para conversion was not considered because of its low capital costs and energy use. The liquefaction system is presented in Fig. 5.

The liquefaction of hydrogen consists of a series of plate and fin heat exchangers and cooling loops with nitrogen pre-cooling and a Claude cooling process [65]. As in [66], hydrogen is introduced to the liquefaction process at 30 bars and $17 \text{ }^\circ\text{C}$ and leaves the process at 2 bars and $-253 \text{ }^\circ\text{C}$. The nitrogen pre-cooling cycle uses 11,110 kmole per hour of

nitrogen and is compressed to 1,100 bar in four compression stages. Most of the compressed nitrogen (95.5%) is expanded and its temperature is reduced to $-195.9\text{ }^{\circ}\text{C}$. The rest of the nitrogen is recycled back into the system. The low temperature stream is used to pre-cool the hydrogen stream that enters the process. In the case of the hydrogen Claude cycle, 39,450 kmole per hour of hydrogen are compressed in three compressors to 70 bars. This

stream is further expanded, cooled, and used for cooling the hydrogen feed. The hydrogen liquefaction plant considers a storage facility. To date, no large-scale facility for liquid hydrogen storage exists but [67] estimated capital costs based on liquefied natural gas (LNG) facilities. The size of the liquid hydrogen tank considered 20 days of storage time which is equivalent to almost 100,000 m^3 of liquid hydrogen.

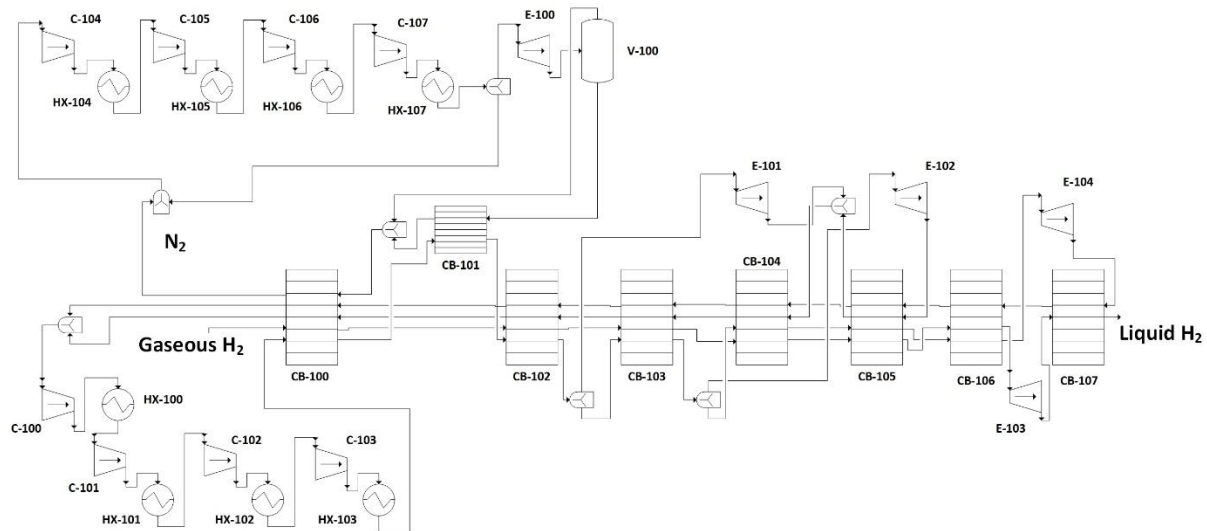


Fig. 5. Hydrogen liquefaction system (see Nomenclature section).

Maritime transport from Orkney to Teesside, pipeline transport to Milford Haven and storage

The direct maritime transport of hydrogen from Orkney was based on the work of [67]. While liquid hydrogen carriers are still in development, there are conceptual designs for 160,000 m^3 carriers and 280,000 m^3 carriers [67-69]. Given the size of the system under analysis, a 160,000 m^3 carrier was selected. Considering the carrier characteristics presented in [67], it was assumed that loading and unloading times were equal and equivalent to 1 day. A round trip from Orkney to Teesside would take in total 82 hours and 10 round trips would be required in a year. A total time of 31 days would be required. The consumption of hydrogen in an engine for propulsion purposes was also estimated considering an efficiency of 35% and a propulsion power of 30 MW [67]. Per voyage, 87 tons of hydrogen are required for propulsion.

For this route, a storage facility with the same characteristics and costs as in Orkney was considered together with a pipeline from Teesside to Milford Haven. The pipeline length is equal to the case of the ammonia pipeline and compression stations were assumed to be placed every 200 km [70]. The pressure drop between each segment is approximately of 10 bar and five compression stations were required. The total duty of

compression was estimated at 4.8 MW. Additionally, four heat exchangers were also considered for reducing the temperature of the compression outlet. The total heat transfer area is 3,318 m^2 with a duty of 3.7 MW. The pipeline transport also includes a regasification terminal at Teesside with cryogenic pumps that increase the hydrogen pressure to 70 bar and heat exchangers that use sea water to evaporate the incoming liquid hydrogen. Given the fact that for LNG facilities 95% of the costs correspond to storage facilities, a shell and tube heat exchanger was considered for regasification of hydrogen [71]. For this, a total heat transfer duty of 14.9 MW was calculated with a heat transfer area of 5,369 m^2 .

Maritime transport from Orkney to Milford Haven and storage

The direct maritime transport of hydrogen from Orkney to Milford Haven and its related costs follow the same procedure as in the previous case. The round trip from Orkney to Milford Haven would take in total 119 hours and 10 round trips would be required, totaling 45 days. For this case, 181 tons of hydrogen would be required for propulsion purposes per roundtrip. In addition to this, regasification facilities were also considered so that hydrogen is delivered at 70 bar and $15\text{ }^{\circ}\text{C}$.

Pipeline transport from Orkney to Milford Haven

For this route, hydrogen produced with the electrolyzer is compressed to 70 bar and transported to the Milford Haven Port through the St. Fergus Gas Terminal and the Teesside Free Port. The total distance for the pipeline was estimated considering the Flotta Oil Terminal in Orkney as the initial point. It was assumed that a 205 km offshore pipeline could transport hydrogen to the St. Fergus Gas Terminal. From this point, and following the existing natural gas infrastructure, a 493 km onshore pipeline could take hydrogen to Teesside and continue to Milford Haven as presented previously. These lengths incorporate a 1.2 factor that takes into account deviations in the pipeline trajectory [51]. It is important to highlight that it is possible that the hydrogen production facilities could be in St. Fergus using offshore wind from a closer location. However, it was not part of this analysis. Additionally, a liquefaction facility in Teesside could be constructed if liquid hydrogen is considered for export to other countries. A compressor of 6.5 MW and a heat exchanger with a duty of 8.6 MW and a heat transfer area of 2,795 m² were calculated for the facilities in Orkney. In addition to this, 9 compression stations were included together with heat exchangers for temperature control. The total duty of the compression stations and heat exchangers are 8.1 MW and 7.7 MW, respectively.

Economic analysis

Based on the systems design presented in the previous sections, the levelized cost of hydrogen was estimated for the entire supply chain. As an initial step, capital costs and operating costs were computed following a detailed analysis of the required process units and the specific conditions of the scenarios under study as presented in the Materials and Methods section.

Ammonia route

Ammonia production (including ASU) and storage at Orkney

Based on the process design presented above, some assumptions need to be taken into account to estimate bare module costs for the different stages in the system under analysis. In the case of ammonia production, and as highlighted by [13], there is no information regarding heat exchanger sizes for operational plants and for this reason overall heat transfer coefficients from several sources of information were revised together with the total estimated heat transfer area [13, 40, 72-74]. In the case of compressors, the electric drive costs were also estimated assuming that an additional 25% of power is needed. The characteristics of the chemical reactor presented above were used to estimate its costs which were similar to the flash drum costs. The

volume of the drums was calculated considering a liquid residence time of 10 minutes [13, 75, 76]. For the purge heat recovery cycle, a boiler, a turbine, and a pump were also included in the cost estimation. Table 3 summarizes the equipment costs and main characteristics calculated with equation 1. Details are presented in Table 2A (Annex).

Table 3. Equipment costs for the ammonia production plant.

Equipment	Design parameters and units	Values	Total cost (million USD)
Ammonia reactor	Volume (m ³)	37.0	19.0
Purge boiler	Duty (MW)	59.0	10.8
Heat exchangers	Area (m ²)	56,803.0	52.8
Flash drums	Volume (m ³)	97.0	24.6
Turbines	Power (MW)	25.9	44.5
Compressors	Power (MW)	29.2	54.1
Pumps	Power (kW)	322.0	2.4
Total			208.2

The bare module costs for the ASU plant were also estimated considering the same equations and procedure presented above. Table 4 presents the main equipment characteristics and costs for the ASU plant calculated with equation 1. Details are presented in Table 3A (Annex). The process considers a compressor train with intercoolers together with a heat exchanger that reduces the temperature of air for the distillation tower. This exchanger is a multi-stream brazed aluminum heat exchanger that uses residual streams for cooling air. Two columns were considered in the design (the high-pressure column and the low-pressure column) together with a turbine and a flash drum. The cost calculations include the heat exchanger and the compressor for N₂ delivery to the ammonia plant.

The costs of a carbon-steel inner tank were estimated considering a material factor of 1.0 and they are 6.6 million USD. The outer tank was estimated with a 1.5 material factor for concrete. For this case, costs were estimated at 12.2 million USD. The compressor (67 kW) for the boil-off recovery system were 0.4 million USD while the condenser costs (102 m²) were 0.3 million USD. The bare module costs for the storage tank were 19.5 million USD. In addition to the latter, a compression train was also added to prepare hydrogen for the required temperature and pressure conditions of the ammonia plant. In this case four compressors and four intercoolers were considered. In the case of the compressors, a total duty of 21.0 MW was estimated with a total cost of 21.7 million USD (including the

electric drives). For the heat exchangers a total area of 3,756 m² was required with total costs of 8.0 million USD.

Table 4. Equipment costs for the ASU plant.

Equipment	Design parameters and units	Values	Total cost (million USD)
Heat exchangers	Area (m ²)	16,763.0	3.9
Cold box	Area (m ²)	98,730.2	15.8
Flash drum	Volume (m ³)	81.4	1.0
Turbine	Power (MW)	0.6	1.1
Compressors	Power (MW)	43.4	41.2
Distillation columns	Volume (m ³)	51.4	1.0
Total			64.0

Considering the bare module costs presented above, for the ammonia production system (including the ASU and the storage facilities and hydrogen compression and heating from the electrolyzer), the *FCI* is equal to 1,217.3 million USD and the *CAPEX* corresponds to 1,399.9 million USD. For the ammonia production system (including the ASU and the storage facilities), the fixed costs (*FC*) are almost 200 million USD per year.

In terms of variables costs, catalysts were considered to be replaced every ten years as mentioned by [68]. This cost was included in the calculations as an investment of 20,384 USD every ten years. Electricity costs were estimated from the LCOE of wind electricity and the corresponding electricity costs and detailed results will be shown later.

Maritime transport from Orkney to Teesside, pipeline transport to Milford Haven and storage

As highlighted by [51], the maritime transport costs include several elements such as the ship chartering rates, port berthing costs, fuel costs and transit fees. These costs are based on the number of voyages per year. It is common practice that energy companies hire external shipping companies and for this reason chartering rates were used [51]. Chartering rates are highly volatile and are highly sensitive to seasonality and other factors including geopolitical events. Several sources of information were revised including those from [77] that estimates rates including specific bunkering and [78] that presents spot market prices for MGCs chartering rates. For the analysis a value of 34,000 USD per day was considered and is based on the weekly average for the second half of 2022 presented by [78]. This value was revised and is similar to the information presented by [51] and [55].

The storage costs for Teesside were calculated following the same procedure and using the same references as in the case of storage facilities in the ammonia production plant. The total bare module costs for this case are 13.0 million USD (lower storage time was considered). Considering equation 7, only equipment erection, piping, instrumentation and electrical were considered. The *CAPEX* in this case corresponds to 28.2 million USD and fixed costs (*FC*) to 5.0 million USD per year.

The costs for the pipeline were taken as 1.1 million USD per km, which corresponds to an average value from [51] and [79]. With this, the pipeline *CAPEX* corresponds to 914.7 million USD with *FC* of 56.0 million USD per year. Finally, storage facilities with the same characteristics as those of the Teesside Free Port were also considered for Milford Haven. Electricity costs were also taken into account (compressors and pumps) and will be presented later.

Table 5. Costs of the main equipment for the ammonia cracking system (including purification).

Equipment	Design parameters and units	Values	Total cost (million USD)
Ammonia cracker	Volume (m ³)	2,500	33.0
Reformer furnace	Duty (MW)	104.6	17.5
Heat exchangers	Area (m ²)	15,968.0	32.5
Cold box	Area (m ²)	59,738.1	16.4
Flash drums	Volume (m ³)	21.2	0.4
Turbines	Power (MW)	15.4	7.9
Compressors	Power (MW)	64.2	114.7
Pumps	Power (kW)	75.5	0.6
Absorption column	Volume (m ³)	93.7	1.8
Total			224.8

Maritime transport from Orkney to Milford Haven and storage

For this transport case, a value of 34,000 USD per day was also considered. In the case of storage, estimated costs were the same as in the case of the Teesside Free Port presented in the previous section.

Ammonia decomposition

Table 5 presents the main equipment sizes together with their costs for the ammonia cracking system calculated with equation 1. Details are presented in Table 4A (Annex). They were estimated following

the same procedure as in the previous parts of the supply chain.

An additional element was considered for the cracking of ammonia (if purification is included) and corresponds to a compression train to deliver hydrogen at pipeline conditions (70 bar and 15°C). For this system six compressors and six intercoolers were incorporated. The compressors have a total duty of 26,767 kW and a total cost of 28.8 million USD, including the electric drives. The intercoolers have a total duty of 23,451 kW and a total area of 11,087 m². The total cost of the intercoolers was 16.9 million USD.

For the ammonia cracking system, the *FCI* is equal to 999.8 million USD and the *CAPEX* corresponds to 1,149.8 million USD. These values correspond to scenarios A and B in which H₂ purification is included. However, for scenario E, purification is not considered. For this scenario, the *FCI* corresponds to 223.0 million USD, while the *CAPEX* is 256.4 million USD. The purification step imposes an important burden to the *CAPEX* because of the refrigeration needed to separate N₂. The fixed costs (*FC*) for the ammonia cracking system with purification are 163.3 million USD per year while these costs are 37.4 million USD per year for the system without purification.

In this case, catalyst costs represent an investment of 55.1 million USD every ten years. For the ammonia cracking system in scenarios A and B, electricity consumption from pumps and compressors was used for estimating variable costs of electricity consumption which will be explained later together with hydrogen production costs. For the ammonia cracking system in scenario E, electricity consumption was not considered since electricity needs are marginal and there is an excess electricity production from the Rankine cycle.

Hydrogen route

Hydrogen liquefaction

For the hydrogen liquefaction plant, Table 6 presents the main equipment sizes together with their costs calculated with equation 1. Details are presented in Table 5A.

With the information from Table 6, the *FCI* was estimated at 989.9 million USD and the *CAPEX* is 1,138.4 million USD. The *CAPEX* for a liquid hydrogen storage facility in Orkney was based on the work of [67] and was estimated at 145.2 million USD and considers cryopumps and the boil-off. The *FC* are 168.040 million USD per year. Electricity costs for the liquefaction plant will be presented at the end of the economic analysis as well.

Maritime transport from Orkney to Teesside, pipeline transport to Milford Haven and storage

The *CAPEX* for a liquid hydrogen carrier was taken from [67] and is equal to 259.8 million USD. The *OPEX* data was obtained from the same previously mentioned source and includes labour costs, maintenance and insurance, corresponding to 3.3 million USD per year. For this route, storage facilities (both in Teesside and Milford Haven) with the same characteristics and costs as in Orkney were considered together with a pipeline from Teesside to Milford Haven. The pipeline costs for transporting hydrogen to Milford Haven were 2 million USD per km. This value corresponds to the average value taken from [70, 81-84]. The *CAPEX* for the pipeline was evaluated in 2,318.7 million USD including compression and regasification costs. The *FC* for this pipeline system was calculated in 140.2 million USD per year. Electricity costs are also presented at the end of the economic analysis.

Table 6. Equipment costs of the main equipment for the hydrogen liquefaction system.

Equipment	Design parameters and units	Values	Total cost (million USD)
Heat exchangers	Area (m ²) [80]	73,786.0	65.9
Cold box	Area (m ²)	276,216.0	54.9
Flash drums	Volume (m ³)	17.7	0.3
Turbines	Power (MW)	26.4	14.7
Compressors	Power (MW)	275.8	132.0
Total			267.8

Maritime transport from Orkney to Milford Haven and storage

The *CAPEX* was the same for this route as presented in the previous section. It includes the maritime transport to Milford Haven, hydrogen storage and regasification facilities. For this route the *CAPEX* is equal to 415.7 million USD. The *FC* for the hydrogen storage and regasification facilities is equal to 3.0 million USD per year.

Pipeline transport from Orkney to Milford Haven

The total cost of the compression stations is 98.3 million USD. The capital costs per km for the onshore pipeline were the same as presented above but for the offshore pipeline, onshore costs were multiplied by a factor of 2.15, that represents the average of low and high estimates according to [71]. In total, the *CAPEX* for the offshore pipeline was 894.9 million USD while the costs for the onshore pipeline were 3,301.2 million USD. The total *CAPEX* for this route is 4,294.4 million USD. For this case, *FC* corresponds to 259.1 million USD per

year. Electricity costs for compression were also considered.

Hydrogen and electricity production costs

At the beginning of the paper, the technical details of the offshore wind and hydrogen production facilities were described. In the case of hydrogen production costs, the *CAPEX* for the PEM electrolyser system was 1,404.4 USD per kW while the *OPEX* was considered a 3% of *CAPEX*. It was assumed that every 7 years stacks need to be replaced and represent 35% of the *CAPEX*. The cost data for the HVDC subsea cable was taken from [29] and a *CAPEX* of 81.6 million USD and an *OPEX* of 1.5% of *CAPEX* were estimated. Water desalination facilities were also incorporated into the calculations with a *CAPEX* of 8.8 million USD (ammonia production system) and 6.5 million USD (liquid and gaseous hydrogen systems). In both cases the *OPEX* represents 3% of *CAPEX*.

The levelized cost of electricity (*LCOE*) was estimated for the offshore wind system using the following equation.

$$LCOE = \frac{CAPEX + \sum_{t=1}^T \frac{OPEX(t)}{(1+r)^t}}{\sum_{t=1}^T \frac{PP(t)}{(1+r)^t}} \quad (11)$$

In equation 11, r is the discount rate, which in this work was taken as 5%, t is the time and T is the useful life of the project (30 years) and PP is the electricity production. For offshore wind, a *CAPEX* of 3,461 USD per kW and an *OPEX* of 74 USD per kW per year were obtained from [85]. With this information an *LCOE* of 59.2 USD per MWh was estimated for average wind conditions. This value together with an average electricity cost of 116.8 USD per MWh (from the grid) were used to evaluate variable costs (VC) for all the stages of the analysed scenarios including the generation of hydrogen in the PEM electrolyser system. The electricity costs for each stage of the supply chains are presented in Table 7.

Levelized cost of hydrogen (LCOH)

The economic information from the previous sections was used to calculate the levelized cost of hydrogen (*LCOH*) using a same formula as equation 11 but adjusted to hydrogen production (PPH) and the *CAPEX* and *OPEX* of each of the stages of the supply chain of the scenarios.

$$LCOH = \frac{CAPEX + \sum_{t=1}^T \frac{OPEX(t)}{(1+r)^t}}{\sum_{t=1}^T \frac{PPH(t)}{(1+r)^t}} \quad (12)$$

Table 7. Electricity costs for every stage in the analyzed processes.

Supply chain stage	Offshore wind (million USD per year)	Grid (million USD per year)
Hydrogen production	278.0	406.1
Ammonia production	23.8	34.8
Maritime transport to Teesside, pipeline	---	0.7
Ammonia route (Scenarios A, B and E)		
Haven and storage		
Maritime transport to Milford Haven and storage	---	0.05
Ammonia decomposition (with purification)	---	74.7
Ammonia decomposition (without purification)	---	---
Hydrogen production	204.1	298.1
Hydrogen liquefaction	67.2	98.2
Hydrogen route (Scenarios C, D, and F)		
Maritime transport to Teesside, pipeline	---	4.9
transport to Milford Haven and storage		
Maritime transport to Milford Haven and storage	---	---
Pipeline transport from Orkney to Milford Haven	1.8	10.1

Figure 6 shows the *LCOH* for the analysed scenarios and for each stage in the supply chain. It must be mentioned that the *LCOH* for hydrogen production varies between the ammonia-based scenarios (A, B and E) and hydrogen scenarios (C, D, and F) because of water desalination costs which depend on hydrogen production quantities. In addition to this, ammonia production and hydrogen liquefaction include storage facilities in Orkney. The results show that Scenario E has the lowest *LCOH* which uses ammonia as an energy carrier but does not consider hydrogen purification (Scenario A is equivalent but includes purification). It must be highlighted that the comparison of hydrogen in Scenario E is not strictly adequate because of its different characteristics in comparison to the other scenarios. However, this result shows that for some applications where highly pure hydrogen is not necessary (for instance combustion), Scenario E is the lowest cost alternative. In this case, nitrogen oxide emissions should be considered and minimized. For applications that require a high purity hydrogen (for instance, fuel cells), hydrogen maritime transport (Scenario C) was the lowest cost scenario in comparison to considering a pipeline in

the UK (Scenario F). High capital costs specially for the offshore part of the pipeline had an important impact on overall costs which could favor the use of the existing natural gas transmission network. In addition to this, combining maritime and pipeline transport presented the highest values of *LCOH*. Finally, Scenario D was more expensive than Scenario B because of the high costs of hydrogen liquefaction, storage and transport along the supply chain. These latter costs were lower in the case of ammonia (Scenario B) which compensate for the high costs of ammonia production, cracking, and hydrogen purification.

Sensitivity analysis

One important aspect that must be highlighted is the fact that most of the stages for the liquefied hydrogen supply chain have not been developed at large-scale and there is a high uncertainty in the values that were used to calculate costs in this and

other studies. While a $\pm 30\%$ error margin is natural for the calculation procedure of all scenarios [7], a sensitivity analysis was performed considering the main variables that could affect the *LCOE* of the scenarios. In this work, changes in the *LCOE* from offshore wind and the electricity costs from the grid were analysed. In the first case, the values of the *LCOE* were adjusted by considering high and low values of the *CAPEX* and the available wind resources through the capacity factor. The *CAPEX* was increased and decreased by 22.3% which corresponds to the standard deviation of data presented by [86]. From the analysis of wind data between 1980 and 2022, a high value capacity factor of 0.61 and a low value capacity factor of 0.54 were also considered. In the case of electricity costs from the grid, a low value of 74 USD per MWh and a high value of 210 USD per MWh were tested.

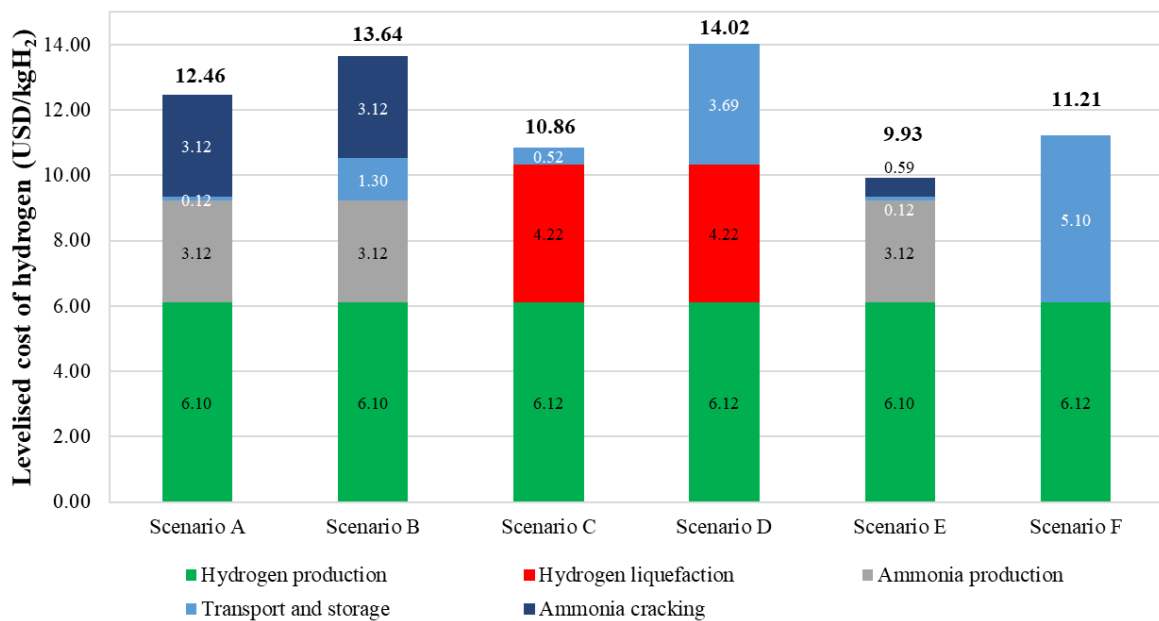


Fig. 6. Levelized cost of hydrogen for the analyzed scenarios.

Figure 7 presents the results from the sensitivity analysis. As observed, the impact of grid electricity costs is larger in comparison to the *LCOE* from offshore wind. The reason for this is the large volatility in electricity costs that highly depend on fossil fuel markets. In addition to this, the scenarios that have a higher consumption of electricity could be impacted by high electricity prices from the grid. This highlights the need for analyzing alternatives such as storage systems that can cope with the intermittency of wind or the addition of base load power generation systems. It is important to mention that the variability in electricity costs had a direct and large effect on hydrogen production.

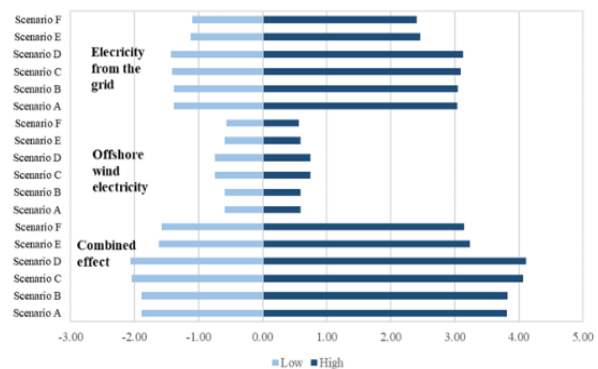


Fig. 7. Sensitivity analysis of the levelized cost of hydrogen.

Discussion and conclusions

The work presented above was aimed at analyzing the techno-economics of ammonia as an energy carrier in the UK. Moreover, the objective was to present a detailed engineering and cost analysis of the alternatives so that this not only complements existing work but provides useful information to translate government plans into reality. In this case, large-scale systems were considered in addition to technologies that could be already deployed or that could be commercially available in the next decade. The design of the processes was revised, and design parameters were within ranges. For instance, the electricity consumption of the Haber-Bosch process which is 0.41 kWh per kg of NH_3 is within the range of values presented by [87]. In addition, costs were also within expected values and, as an example, the ammonia cracking system CAPEX is 4.1 million USD per tonne of ammonia per day which is within the values presented by [7] and [8]. The results show that ammonia is a cost-efficient energy carrier together with its decomposition back to hydrogen when this latter compound is not purified. This highlights the need to further analyze the techno-economics of these systems considering the final use of hydrogen or ammonia. The consideration of these fuels as alternatives for the decarbonization of the economies needs to be analyzed from a supply and demand perspective. This work also highlights the need to consider the regional aspect of projects which will influence the solution. The use of ammonia as an energy carrier is a feasible solution that has been used for several decades with proven technology. Despite of this, the environmental impacts (not only NH_3 slip emissions but nitrogen oxide emissions from combustion) and safety concerns should be analyzed in more depth together with its local acceptance [88]. With regards to the latter, while already established industrial areas were selected for ammonia production and cracking, it is important to further analyze these concerns for the specific locations of its transport, storage and use. These factors may also have an important impact on the final costs and feasibility of a green ammonia project. In addition to this, in the case of hydrogen, most of the process stages presented in this work have not been tested yet, which increase the uncertainty in cost estimations. While they could reach an advanced stage of development in the future, the implementation of low-carbon solutions cannot wait, and ammonia can fill this gap. As a final point it is important to consider that the systems under analysis incorporate electricity from the grid which is still generated by fossil-based technologies adding GHG emissions to ammonia and hydrogen. For this reason, it is necessary to study energy storage and other base-load low-carbon electricity

sources that could cope with the intermittency of renewable energy sources in the

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Conflicts of Interest

The authors declare no conflict of interest. The funders had no role in the design of the study; in the collection, analyses, or interpretation of data; in the writing of the manuscript, or in the decision to publish the results.

Nomenclature

Abbreviation or symbol	
C-	Compressor
C_1	Costs for equipment with capacity S_1
C_2	Costs for equipment with capacity S_2
CB-	Cold box
C_{Bmi}	Bare module costs for equipment i
DESNZ	UK Department of Energy Security and Net Zero
E-	Expander
f	Correction factor for ammonia synthesis
FC	Fixed costs
FCI	Fixed capital investment
F-	Furnace
HX-	Heat exchanger
IPC	Indirect plant costs
k_1	Pre-exponential factor for the ammonia synthesis forward reaction
k_2	Pre-exponential factor for the ammonia synthesis reverse reaction
k_3	Pre-exponential factor for the ammonia cracking reaction
$LCOE$	Levelized cost of electricity
$LCOH$	Levelized cost of hydrogen
NP	Number of non-particulate stages
P-	Pump
PP	Electricity production
PPC	Direct plant costs
PPH	Hydrogen production
r	Discount rate
R-	Reactor
r_{N_2}	Rate of reaction for nitrogen in ammonia synthesis
r_{NH_3}	Rate of reaction for ammonia in ammonia cracking
S_1	New equipment capacity
S_2	Existing equipment capacity
T-	Column
V-	Flash tank
VC	Variable costs
WC	Working capital
Greek symbol	
α	Constant for economies of scale
β	Reaction coefficient. Ammonia cracking
ρ_{cat}	Catalyst bulk density

Annex

Table A1. Equipment constants for equation 1 [13, 14].

Equipment	K_1	K_2	K_3
Heat exchanger (HX-)	4.8306	-0.8509	0.3187
Reactor (R-), Flash tank (V-) or Column (T-)	3.4974	0.4485	0.1074
Reciprocating pump (P-)	3.8696	0.3161	0.122
Centrifugal compressor (C-)	2.2897	1.3604	-0.1027
Compressor electric drives (C-)	1.956	1.7142	-0.2282
Expander (E-)	2.2476	1.4965	-0.1618
Furnace (F-)	7.3488	-1.166	0.2028

Table A2. Bare module costs for the ammonia synthesis plant equipment.

Equipment	Characteristics	Cost (Million USD)
Heat exchangers		
Cooler between bed 1 and 2 of the ammonia reactor (HX-100).	The heat transfer area was 809 m ² and a heat transfer coefficient of 60 W/m ² K was considered [40]. The required duty was 20.2 MW.	2.1
Cooler between bed 2 and 3 of the ammonia reactor (HX-101).	The heat transfer area was 292 m ² and a heat transfer coefficient of 60 W/m ² K was considered [40]. The required duty was 7.8 MW.	0.9
Heat exchanger for the recycle for bed 1 of the ammonia reactor (HX-102).	The heat transfer area was 2,293 m ² and a heat transfer coefficient of 200 W/m ² K was considered [40]. The required duty was 41.5 MW.	4.3
Heater for the syngas recycle to enter the process (HX-103).	The heat transfer area was 1,698 m ² and a heat transfer coefficient of 200 W/m ² K was considered [40]. The required duty was 46.7 MW.	3.6
Heat exchanger for the boil-off recycle and the reactor product cooling (HX-104).	The heat transfer area was 529 m ² and a heat transfer coefficient of 200 W/m ² K was considered [40]. The required duty was 34.3 MW.	1.4
Ammonia cooler (HX-105).	The heat transfer area was 38,210 m ² and a heat transfer coefficient of 500 W/m ² K was considered [13]. The required duty was 95.8 MW.	23.4
Ammonia cooler (using the refrigeration cycle) (HX-106).	The heat transfer area was 3,842 m ² and a heat transfer coefficient of 865 W/m ² K was considered [13]. The required duty was 60.7 MW.	5.9
Compressor intercoolers for the refrigeration cycle (HX-107, HX-108, HX-109).	To reduce the temperature within the compressor train and increase efficiency, three intercoolers were integrated. It was assumed that water was the cooling medium. For this reason, a heat transfer coefficient of 60 W/m ² K was used [40]. The total heat transfer area was 1,524 m ² .	2.8
Condenser in the refrigeration cycle (HX-110).	The heat transfer area was 2,517 m ² and a heat transfer coefficient of 500 W/m ² K was considered [13]. The required duty was 75.3 MW.	3.1
Condenser in the Rankine cycle (HX-111).	The heat transfer area was 3,392 m ² and a heat transfer coefficient of 1,250 W/m ² K was considered [72]. The required duty was 78.9 MW.	2.4
Heat exchanger for boil-off combustion flue gases (HX-112).	The heat transfer area was 430 m ² and a heat transfer coefficient of 160 W/m ² K was considered [72]. The required duty was 32.1 MW.	0.9
Heat exchanger for boil-off flue gases (waste heat recovery) (HX-113).	The heat transfer area was 749 m ² and a heat transfer coefficient of 160 W/m ² K was considered [72]. The required duty was 9.7 MW.	1.4
Condenser in the boil-off combustion Rankine cycle (HX-114).	The heat transfer area was 518 m ² and a heat transfer coefficient of 1,250 W/m ² K was considered [72]. The required duty was 33.0 MW.	0.6

Compressors		
Synthesis gas recycle compressor (C-100).	Increases the pressure of the recycle to feed conditions. The total duty of the compressor was 1,153 kW.	4.1
Compressor train of the refrigeration cycle (C-101, C-102, C-103, C-104).	The total duty of the four compressors was calculated in 28,032 kW.	50.0
Ammonia reactor and flash drums		
Reactor (R-100, R-101, R-102).	The three beds have a total volume of 37 m ³ and costs were adjusted considering operating pressures and materials.	19.0
Flash drums (V-100, V-101).	In this work, two flash drums were considered. The volume of each drum was 51.5 m ³ and 45.3 m ³ .	24.6
Heat recovery		
Purge boiler (F-100).	In this case a chemical equilibrium reactor and a furnace efficiency of 85% was considered. Its duty was 58,974 kW [72].	10.8
Turbine (purge) (E-101).	The duty of the turbine was 8,842 kW. Cost adjustments were estimated using [72].	4.9
Reciprocating pump (purge) (P-101).	The duty of the pump corresponded to 97 kW and costs were estimated following [13].	0.8
Turbine (Rankine cycle for ammonia cooling) (E-100).	The duty of the turbine was 17,070 kW. Costs adjustments were estimated using [72].	39.6
Reciprocating pump (Rankine cycle for ammonia cooling) (P-100).	The duty of the pump corresponded to 225 kW and costs were estimated following [13].	1.6
Total costs		208.2

Table A3. Bare module costs for the ASU equipment.

Equipment	Characteristics	Cost (Million USD)
Heat exchangers		
Air compressor intercoolers (HX-100, HX-101, HX-102).	The heat transfer areas for the three intercoolers were 5,796 m ² , 5,839 m ² and 4,979 m ² . The heat transfer coefficient of 60 W/m ² K was considered [40]. The required duty was 32.9 MW.	3.3
Cold box heat exchanger (CB-100).	The area of this heat exchanger was calculated following the procedure and assumptions taken from [13] and [50]. The total heat duty of the cold box is 34.6 MW.	15.8
Nitrogen heater for ammonia plant (HX-103).	The heat transfer area was 149 m ² and a heat transfer coefficient of 160 W/m ² K was considered [72]. The required duty was 2.4 MW	0.6
Compressors		
Compressor train for the air feed (C-100, C-101, C-102).	The total duty of the four compressors was calculated in 34,980 kW.	26.8
Nitrogen compressor for ammonia plant (C-103).	The total duty of compressor calculated in 8,391 kW.	14.4
Distillation columns		
High pressure column (HPC) (T-100).	The design was based on the work of [13], [46] and [50] but it was adjusted to the process conditions in this work, considering the sizing equations from [76]. A total volume of 22.3 m ³ was estimated for this column.	0.6
Low pressure column (LPC) (T-101).	The design was based on the work of [13], [46] and [41] but it was adjusted to the process conditions in this work, considering the	0.4

	sizing equations from [76]. A total volume of 29.1 m ³ was estimated for this column.	
Flash drums and turbines		
Flash drum (V-100).	The flash drum was calculated considering stainless steel as its material of construction and that it operates at 1.3 bar with the same procedures as the flash drums in the ammonia synthesis plant.	1.0
Turbine (E-100).	The duty of the turbine was 636 kW. Costs adjustments were estimated using [72].	1.1
Total costs		64.0

Table A4. Bare module costs for the ammonia cracking plant equipment.

Equipment	Characteristics	Cost (Million USD)
Heat exchangers		
Ammonia vapouriser (HX-100).	The heat transfer area was 119 m ² and a heat transfer coefficient of 1,275 W/m ² K was considered [72]. The required duty was 38.4 MW.	0.4
Ammonia heater for reactor (HX-101).	The heat transfer area was 290 m ² and a heat transfer coefficient of 200 W/m ² K was considered [13]. The required duty was 13.4 MW.	0.6
Air heater for cracker (HX-102).	The heat transfer area was 1,013 m ² and a heat transfer coefficient of 165 W/m ² K was considered [80]. The required duty was 13.4 MW	1.9
Cracker product cooler (Rankine cycle) (HX-103).	The heat transfer area was 974 m ² and a heat transfer coefficient of 1,250 W/m ² K was considered [80]. The required duty was 36.6 MW.	1.9
Compressor intercoolers (before absorption column) (HX-105, HX-106, HX-107).	It was assumed that water was the cooling medium. For this reason, a heat transfer coefficient of 60 W/m ² K was used [13]. The total heat transfer area was 5,545 m ² with a duty of 15.4 MW.	12.5
Compressor intercoolers for N ₂ separation (HX-108, HX-109, HX-110, HX-111, HX-112).	It was assumed that water was the cooling medium. For this reason, a heat transfer coefficient of 60 W/m ² K was used [13]. The total heat transfer area was 7,282 m ² with a duty of 46.2 MW.	13.8
Condenser for the Rankine cycle (HX-104).	The heat transfer area was 745 m ² and a heat transfer coefficient of 1,250 W/m ² K was considered [80]. The required duty was 29.7 MW.	1.4
Cold box heat exchanger for N ₂ separation (CB-100).	The area of this heat exchanger was calculated following the procedure and assumptions taken from [13] and [50]. The total heat duty of the cold box is 20.9 MW.	16.4
Compressors		
Compressor train before absorption column (C-100, C-101, C-102).	The total duty of the three compressors was 15,007 kW.	31.4
Compressor train for N ₂ separation (C-103, C-104, C-105, C-106, C-107, C-108).	The total duty of the six compressors was calculated in 49,159 kW.	83.3
Ammonia cracker and flash drums		
Reactor (R-100).	The three beds have a total volume of 2,500 m ³ and costs were adjusted considering operating pressures and materials.	33.0
Furnace (F-100).	In this case a chemical equilibrium reactor was considered. Its duty was 104,600 kW which is the energy required by the cracker. For this case, carbon steel is considered as the material for the boiler [72].	17.5
Flash drums (V-100, V-101).	In this work, two flash drums were considered. The volume of each drum was 0.1 m ³ and 21.1 m ³ .	0.4
Ammonia separation		

Absorption column (T-100).	The absorption column was designed considering equilibrium and using the Kremser equation [7, 73]. The number of estimated stages was 16. The estimated diameter was 3.3 m and a volume of 93.7 m ³ . The height of the column is 11.2 m.	1.8
Turbines and pumps		
Turbine in the Rankine cycle (E-100).	The duty of the turbine was 6,965 kW. Costs adjustments were estimated using [72].	2.9
Turbine for water separation (E-101).	The duty of the turbine was 5,568 kW. Costs adjustments were estimated using [72].	2.8
Turbine for N ₂ separation (E-102).	The duty of the turbine was 2,861 kW. Costs adjustments were estimated using [72].	2.2
Reciprocating pumps (P-100, P-101).	Two pumps were considered, and their duty corresponded to 1.0 kW (ammonia) and 74.5 kW (Rankine cycle) [13].	0.6
Total costs		224.8

Table A5. Bare module costs for the hydrogen liquefaction plant equipment.

Equipment	Characteristics	Cost (Million USD)
Heat exchangers		
Compressor coolers for the hydrogen Claude cycle (HX-100, HX-101, HX-102, HX-103).	To reduce the temperature within the compressor train and increase efficiency, three intercoolers were integrated together with a heat exchanger for the last compressor. It was assumed that water was the cooling medium. For this reason, a heat transfer coefficient of 60 W/m ² K was used [13]. The total heat transfer area was 53,024 m ² with a total duty of 165.3 MW.	37.0
Compressor coolers for the nitrogen pre-cooling cycle (HX-104, HX-105, HX-106, HX-107).	To reduce the temperature within the compressor train and increase efficiency, three intercoolers were integrated together with a heat exchanger for the last compressor. It was assumed that water was the cooling medium. For this reason, a heat transfer coefficient of 60 W/m ² K was used [13]. The total heat transfer area was 20,762 m ² with a total duty of 100.0 MW.	28.9
Heat exchanger 1 (CB-100).	The area of this heat exchanger was calculated following the procedure and assumptions taken from [13] and [50]. The total heat duty of the heat exchanger is 75.6 MW with a total heat transfer area of 216,032 m ² .	32.2
Heat exchanger 2 (CB-101).	The area of this heat exchanger was calculated following the procedure and assumptions taken from [13] and [50]. The total heat duty of the heat exchanger is 2.4 MW with a total heat transfer area of 6,745 m ² .	2.9
Heat exchanger 3 (CB-102).	The area of this heat exchanger was calculated following the procedure and assumptions taken from [13] and [50]. The total heat duty of the heat exchanger is 5.0 MW with a total heat transfer area of 14,373 m ² .	5.0
Heat exchanger 4 (CB-103).	The area of this heat exchanger was calculated following the procedure and assumptions taken from [13] and [50]. The total heat duty of the heat exchanger is 1.2 MW with a total heat transfer area of 3,518 m ² .	1.9
Heat exchanger 5 (CB-104).	The area of this heat exchanger was calculated following the procedure and assumptions taken from [13] and [50]. The total heat duty of the heat exchanger is 1.3 MW with a total heat transfer area of 3,750 m ² .	1.9

Heat exchanger 6 (CB-105).	The area of this heat exchanger was calculated following the procedure and assumptions taken from [13] and [50]. The total heat duty of the heat exchanger is 7.6 MW with a total heat transfer area of 21,825 m ² .	6.6
Heat exchanger 7 (CB-106).	The area of this heat exchanger was calculated following the procedure and assumptions taken from [13] and [50]. The total heat duty of the heat exchanger is 2.2 MW with a total heat transfer area of 6,352 m ² .	2.8
Heat exchanger 8 (CB-107).	The area of this heat exchanger was calculated following the procedure and assumptions taken from [13] and [50]. The total heat duty of the heat exchanger is 1.3 MW with a total heat transfer area of 3,621 m ² .	1.6
Compressors		
Compressor train for the nitrogen pre-cooling cycle (C-104, C-105, C-106, C-107).	The compressor train includes four compressors with duties of 22.3 MW, 23.0 MW, 23.6 MW and 29.8 MW.	55.1
Compressor train for the hydrogen Claude cycle (C-100, C-101, C-102, C-103).	The compressor train includes four compressors with duties of 53.9 MW, 58.5 MW, 47.3 MW and 17.4 MW.	76.9
Flash drums and turbines		
Flash drum (V-100).	The flash drum has a volume of 17.7 m ³ and was calculated with the same procedures as the flash drums in the other processes.	0.3
Turbine in the nitrogen pre-cooling cycle (E-100).	The duty of the turbine was 19,440 kW. Costs adjustments were estimated using [72].	7.9
Turbine 1 in hydrogen cooling cycle (E-101).	The duty of the turbine was 596 kW. Costs adjustments were estimated using [72].	1.0
Turbine 2 in hydrogen cooling cycle (E-102).	The duty of the turbine was 1,142 kW. Costs adjustments were estimated using [72].	1.5
Turbine 3 in hydrogen cooling cycle (E-103).	The duty of the turbine was 441 kW. Costs adjustments were estimated using [72].	0.9
Turbine 4 in hydrogen cooling cycle (E-104).	The duty of the turbine was 4,762 kW. Costs adjustments were estimated using [72].	3.4
Total costs		267.8

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