Process implications of electrifying ammonia production

[a] Antoine Dechany, [b] Kevin Van Geem, [a*] Joris Proost
[a] Université catholique de Louvain, Division of Materials and Processes Engineering, Place Sainte-Barbe 2, Louvain-la-Neuve, Belgium
[b] Universiteit Gent, Laboratory for Chemical Technology, Technologiepark 125, B-9025, Ghent, Belgium

*Corresponding author e-mail: joris.proost@uclouvain.be

Abstract

Current ammonia production, based on Steam Methane Reforming (SMR) coupled to the Haber-Bosch (HB) process, are responsible for about 1,2% of global CO2 emissions. Therefore, also the NH3 industry is considering a full or partial electrification, e.g. by replacing SMR-based by electrolytic H2 production. This paper critically considers the implications of such a shift for 2 alternative scenarios, namely combining HB with either low- or high-temperature electrolysis. Regarding emissions, electrification can indeed be beneficial with a cut of up to 96-99%, but only when using 100% renewable electricity rather than a coupling to the currently still mainly fossil-driven grid. Also energy efficiency can be improved, thanks to the availability of high purity electrolytic hydrogen and electrical rather than steam-based compressors. However, due to the higher intrinsic energy demand of electrolytic H2, the total energy consumption (in GJ/tonne NH3) for both alternative scenarios exceeds that of the conventional process.

Keywords: Ammonia, Haber-Bosch, Electrolysis, Electrification, Hydrogen, CO_2 emissions

Introduction

There is no doubt that the climate crisis is the number one issue the world has to tackle. As a consequence, paradigm shifts are happening globally to reduce greenhouse gas emissions, be it on small scales such as in individuals' routines, or on larger scales such as in the transport, building, power and industrial sector. Looking closer at the chemical sector, it was responsible for 1,4 $GtCO_2$ in 2019, which is equivalent to 4,2% of global CO_2 emissions [1,2]. Within those 4,2%, 1,2% are attributable to ammonia production and its methane-based Haber-Bosch (HB) process, making it one of the largest greenhouse gas emitters within the chemical sector [3,4]. Solutions to reduce its carbon footprint could therefore have a significant impact on global emissions. Recently, electrification has been one of the main focuses when assessing decarbonizing solutions for different sectors [5], and the chemical industry is one of the most crucial. Several studies have assessed the electrification of NH_3 production by replacing Steam Methane Reforming (SMR) for H_2 production by water electrolysis [3,4,6]. As a matter of fact, the original idea was already formulated as far back as 1925 [7], at a time when SMR technology was not available yet. The first plant with an alkaline electrolyser was built by Norsk Hydro in 1981 [8]. Today, a few pilot plants already exist such as one in Oxford (20 kg/day) and Fukushima (30 kg/day) [9]. The Norwegian company Yara has teamed up with ENGIE to build a commercial plant by 2023

(10137 kg/day) [10], while Haldor Topsøe has constructed an ammonia synthesis plant fed with hydrogen produced via Solid Oxide Electrolysis [11].

Implementing such a change in H_2 production technology also implies significant changes in the whole process. The main objective of this work is to critically review these implications by comparing three scenarios in terms of energy consumption and CO_2 emissions. The base case is the current Best Available Technology for NH_3 production: the combination of SMR and HB. The first and second alternatives will then replace SMR by low- and high-temperature water electrolysis, respectively.

Scenario description

Scenario 0: Steam Methane Reforming (SMR) + Haber-Bosch (HB)

Scenario 0 is the name given to the reference scenario as it describes the current situation. Ammonia is produced through a high-temperature and high-pressure catalytic process called Haber-Bosch, which is fed with a H_2/N_2 mixture produced by Steam Methane Reforming (Fig. 1a). The combination of the SMR reactions (1) and (2) (reaction 1 for the reforming step and reaction 2 for the water gas shift) with the Haber-Bosch reaction (3) currently represents the Best Available Technology (BAT) for NH_3 production as it yields the highest efficiency and lowest carbon emissions while being the most economical route for large scale NH_3 production [3,12]. Typical operating conditions for each step in the process are given in Table 1.

$$CH_{4(g)} + H_2O_{(g)} = CO_{(g)} + 3H_{2(g)} \ ; \ \Delta H^0 = 206 \text{ kJ} \tag{1}$$

$$CO_{(g)} + H_2O_{(g)} = CO_{2(g)} + H_{2(g)}; \ \Delta H^0 = -41 \text{ kJ} \tag{2}$$

$$N_{2(g)} + 3H_{2(g)} = 2NH_{3(g)} \ ; \ \Delta H^0 = -92{,}4 \text{ kJ} \tag{3}$$

Scenario 1 : Low-temperature electrolysis (Alkaline Electrolysis or Proton Exchange Membrane Electrolysis) + Haber-Bosch (HB)

One of the main drawbacks of the conventional scenario is its reliance on fossil fuel (methane) for the H_2 production. A solution to tackle this issue is the implementation of an electrical alternative. One of the most studied technologies are Water Electrolysers (WE) which can produce hydrogen via reaction (4) [13,14]. The reaction is powered electrically and, given that the electricity comes from renewable sources, the resulting hydrogen can be qualified as green H_2 [15].

$$H_2O_{(liq)} = H_{2(g)} + \tfrac{1}{2}\, O_{2(g)} \ ; \ \Delta H^0_{liq} = 286{,}0 \text{ kJ} \tag{4}$$

O_2 is also produced but as a by-product of no direct use in the synthesis of ammonia. It can be stored and used in other applications such as blast furnaces, glass melting and medical applications [16]. In order for WE to replace SMR in an ammonia production plant, as it only produces H_2 and O_2, nitrogen should be provided by an Air Separation Unit (ASU), usually cryogenic distillation or pressure swing adsorption (PSA) [17,18].

Several technologies exist when considering WE, and they are usually distinguished by their operating temperatures. In Scenario 1, a low-temperature electrolyser is used (Fig. 1.b), typically Alkaline Electrolyser (AE) or Proton Exchange Membrane Electrolyser (PEME). The purity of the hydrogen produced is ranging between 99,5% (AE) up to 99.99% (PEME). Both technologies operate at a similar electric efficiency between 60 and 70% based on the LHV of hydrogen [19–21]. Overall, AE has a Technology Readiness Level (TRL) of 9 while PEME is at 8-9 [18]. The required operating conditions are gathered in Table 1.

Scenario 2: High-temperature electrolysis (Solid Oxide Electrolysis) + Haber-Bosch (HB)

In Scenario 2, high-temperature electrolysis is considered by using a Solid Oxide Electrolyser (SOE) (Fig. 1.c), working at a similar pressure range as AE but at much higher temperatures (cfr. Table 1). Due to temperature surpassing 100°C, the water feed is in vapor state, which has a lower standard enthalpy compared to liquid water (cfr. reaction (5)).

$$H_2O_{(g)} = H_{2(g)} + \frac{1}{2} O_{2(g)} \ ; \ \Delta H^0_g = 241{,}8 \text{ kJ} \qquad (5)$$

This makes the coupling of SOE with HB interesting as it allows to recover waste heat from the Haber-Bosch unit, avoiding additional heat sources. The produced hydrogen can reach a purity of 99,9% with high electric efficiencies around 82% [11,20]. In terms of technology readiness, SOE are still in an early development stage with a TRL of 5-6 [18].

Results & discussion

To evaluate the implications of electrifying ammonia production and compare the different scenarios, two characteristics are assessed: energy consumption and CO2 emissions. Values presented below have been gathered from the existing literature.

Energy consumption

For each scenario, the energy consumption is broken down by units on Figure 2. Each scenario has a theoretical minimum consumption as well as energy losses.

Theoretical minimum energy consumption

It is important to first clarify the method for calculating the theoretical minimum, since quite some confusion exists in the literature. For the reference case (SMR + HB), the minimum energy required is usually calculated based on the heat of combustion (LHV) of methane [22–24]. By multiplying the amount of methane needed to synthesize 1 ton of ammonia (353 kg/tNH3) by the LHV of methane (50 MJ/kg), a theoretical consumption of 17,7 GJ/tNH3 is then obtained. Added to that the heat to be supplied to the furnaces for driving the endothermic reforming reactions (4,5 GJ/tNH3 [22]), the minimum energy consumption amounts to 22,2 GJ/tNH3 [22].

However, as already pointed out by Sohn et al. [25], using the heat of combustion of methane as a basis for energy consumption calculations is quite doubtful, as the methane feedstock is not burnt but transformed into H2. In our opinion, a more relevant method would be to use the standard reaction enthalpy of the global reforming reaction, obtained by summing up reactions (1), (2) and (3) as follows:

$$3CH_{4(g)} + 6H_2O_{(l)} + 4N_{2(g)} = 3CO_{2(g)} + 8NH_{3(g)} \text{ ; } \Delta H^0 = 125{,}4 \text{ kJ} \qquad (6)$$

This gives a value of ΔH° = 125,4 kJ, corresponding to 0,9 GJ/tNH3. Added to the furnace heat, the theoretical minimum would then rather be equivalent to 5,4 GJ/tNH3, a value that is 4 times smaller than the one currently considered in the literature. Obviously, by doing so, the assumption is made that an ideal heat recycling (i.e. no heat loss) can be implemented between the exothermal WGS and HB reactions (2) and (3) on the one hand, and the endothermal reforming reaction (1) on the other hand. This assumption is not valid for the current NH_3 production process since the excess heat from the HB reactor is currently used to generate steam for driving the compressors (cfr. Fig. 1.a). However, this could be adapted in the future by replacing the steam turbines in the compressors with electrical motors.

For both alternative scenarios, the minimum energy consumption is usually calculated as well based on the global standard reaction enthalpy, as obtained by summing up reactions (3) and (4) or (5):

$$3H_2O_{(liq/gas)} + N_{2(g)} = \frac{3}{2} O_{2(g)} + 2NH_{3(g)} \text{ ; } \Delta H^0_{liq} = 765{,}6 \text{ kJ, } \Delta H^0_{gas} = 633 \text{ kJ} \qquad (7)$$

Once again, the resulting reaction can be seen as an ideal summary of the whole process, where the heat from the exothermal reactions is perfectly recycled to the endothermal electrolysis reaction. In Scenario 1 (AE), the standard enthalpy of reaction (7) is 765,6 kJ, corresponding to a theoretical minimum consumption of 22,5 GJ/tNH3. It should be kept in mind that the assumption has limitations, as in reality the HB heat cannot be entirely recycled to the AE due to the low operating temperature of the latter (cfr. dashed red arrow in Fig. 1.b). In Scenario 2 however, SOE can effectively be fed with the recovered heat from the HB section [6]. Moreover, due to the high operating temperatures of the SOE, water is present as steam which decreases the electrolysis enthalpy. As a result, the enthalpy of reaction (7) is decreased to $\Delta H^0 = 633$ kJ, corresponding to a theoretical minimum consumption of 18,6 GJ/tNH3. Note that both values are in fair agreement with the ones given by Smith et al. [4], namely 21,1 and 18,7 GJ/tNH3 for AE and SOE-based ammonia production, respectively.

Energy loss

Electrification not only has an impact on the theoretical minimum energy consumption, but also on the energy efficiency of the entire process. A direct implication is a cut in the energy losses from the Haber-Bosch loop. This is due to a combination of two factors. The first one is the high purity of the mix produced by the electrolysis and air separation unit, containing less than 0,2 vol% of argon. As this amount is soluble in NH_3, the purge is not necessary anymore and can be removed, allowing to spare 16% of the energy losses [23,26]. This purity also results in lower compression energy, as the inert gases will less dilute the H_2/N_2 mix. The second factor is the electrification of the compressors. In conventional plants, compressors are driven with steam turbines. The latter operate with a 45% efficiency and are responsible for 55-60% of all losses (6,6 GJ/tNH3) [4]. Replacing them with electrical motors, which work at much higher efficiencies (95%), would allow to spare 3,1 GJ/tNH3 of compression energy loss. The topic of steam turbine replacement with electrical motors could lead to a significant change in the design of the compressors. In the context of ammonia production, such a replacement already occurred in 1985 by BASF which successfully revamped an ammonia plant with minimal fitting and aligning of the motors once installed [27]. This topic is also of generic interest as quite a few process industries are trying to tackle the design challenges associated with electrifying steam-driven installations [28].

Electrification of the compressors also affects the heat integration of the Haber-Bosch reactor. In the conventional case, the heat removed from the reactor is recovered via inter-stage cooling and used to produce steam for the H_2/N_2 compressor. The use of electrical motors instead of steam turbines makes such heat integration useless in Scenario 1, while it is redirected to the SOE in Scenario 2 (cfr. Fig. 1c.). In the former case, a redesign of the HB reactor could be interesting to implement inter-stage cooling and optimize the reaction condition. Cheema *et al*. already studied such a redesign for autothermal ammonia production [29]. In latter case, considering the heat requirement of SOE to be 3,5 GJ/tNH3 [6], the heat recycled from the HB process (2.7 GJ/tNH3) provides only 77% of the SOE requirements [17], still leaving 0,8 GJ/tNH3 to be provided by an external heat source. Note that this is fundamentally different from the analysis in ref. [6], where as a result of an unrealistically high operating temperature for HB of 650°C, a heat recovery of 3.44 GJ/tNH3 is claimed.

While electrification clearly results in an improved energy efficiency of the ammonia production and the compression system, hydrogen production now becomes the main source of energy loss. In Scenario 1, 9,7 GJ/tNH3 of loss originates from the AE stack only, given its 70% efficiency. This value is lower in Scenario 2 as SOE operates at a higher efficiency (82%). In the latter case, the energy loss would be dominated by compression, similar to Scenario 0, at least if we take the value of 5,8 GJ/NH3 given by Cinti et al. [6], based on a rather high inlet pressure of 550 bar at the HB reactor. Finally, the Air Separation Unit introduced in the electrified scenario is a new source of energy losses. These losses depend on the chosen technology [11]. In the case of Pressure Swing Adsorption (PSA), 0,7 to 1,0 GJ/tNH3 are lost [18].

CO_2 emissions

CO_2 emissions for each scenario are compared in Figure 3. As can be expected, the emissions are much higher in the conventional methane-fed case, emitting a total of 2,33 tCO2/tNH3. Most of the emissions originate from the use of methane, either as feedstock for SMR (1,13 tCO2/tNH3) or as fuel for the furnace (0,41 tCO2/tNH3) [4,30]. Methane extraction and infrastructure emissions amount to 0,33 tCO2/tNH3 [9]. Finally, the steam system and heat losses emit 0,30 and 0,17 tCO2/tNH3 respectively. Even when considering the most optimized and efficient plants plus the methane extraction and transport, there is still 1,8 tCO2/tNH3 as reported by Wang et al. [9]. The latter went further by describing a theoretical scenario implementing a Carbon Capture and Storage (CCS) unit, which would further decrease the emissions to 0,5 tCO2/tNH3.

In comparison, both electrified scenarios do not emit any amount of CO_2 directly and therefore have a much lower carbon footprint [31], depending on the footprint of the electricity source used to drive the electrical units (electrolyser, ASU and compressors). To have a comprehensive overview on the impact of the electricity source, four different cases were considered : the electricity grid in 2020, the projected grid in 2030, wind electricity and hydroelectricity. As can be seen in Fig. 3, the first 2 scenarios would not be much better in terms of emissions considering today's fossil carbon-based electricity, which in Europe emits 231 g/kWh and are predicted to decrease to 118 g/kWh in 2030 in the most pessimistic scenario [32]. Assuming the use of renewable energies as in Smith et al. [4], total emissions would not reach more than 0,09 tCO2/tNH3 for wind and 0,03 tCO2/tNH3 for hydropower, meaning an emission reduction equivalent to 96,1% and 99,1% respectively. In both cases, the emissions are linked to the production, transport and building of the wind turbines, dams, dikes and power stations. These values were calculated following Raadal et al., who detailed the footprints of several types of wind turbines (10,4 g/kWh for 1-5 MW turbines) and hydropower plants (2,9 g/kWh) [33]. For further reading on the carbon footprint of electricity sources, Tackett *et al.* provided a nice analysis on how this crucial point needs to be taken into account during CO_2 to methanol conversion [34].

Conclusions

In this paper, the process implications of electrifying ammonia production have been critically reviewed. Three scenarios were considered and compared in terms of energy efficiency and CO_2 emissions. For the latter, both the integration of AE and SOE allow for a significant reduction in the CO_2 emissions (up to 96-99%), provided that the electricity is supplied by renewable electricity. Using the current (2020-2030) electricity grid is still too fossil carbon intensive and would result in a similar footprint compared to the current situation. Conclusions are more ambiguous when it comes to energy efficiency. First and foremost, the usual calculation method for the theoretical minimum energy consumption (based on the LHV-value of methane) has been questioned. Instead, the LHV value has been replaced by a thermodynamic more sound quantity being the reaction enthalpy. Electrification does allow to decrease the energy consumption, mainly thanks to the use of high purity electrolytic hydrogen, which permits the suppression of a purge in the HB process, and also the replacement of steam turbines with more efficient electrical compressors. However, due to the higher intrinsic energy demand of electrolytic H2, the total energy consumption (in GJ/tonne NH3) for both alternative scenarios is higher compared to that of the conventional process. Finally, the heat integration strategy needs complete revision in both alternative scenarios. In Scenario 1, most of the heat generated by the HB process needs to be recycled elsewhere as AE is a low-temperature process. This could be done by re-designing the HB reactor for optimized inter-stage cooling. In Scenario 2, this excess heat can be sent to the high-temperature SOE.

Acknowledgements

Funding from the Belgian Energy Transition Funds of the Federal Planning Service for Economy, S.M.E., Self-employment and Energy is gratefully acknowledged through the BE-HyFE project (Belgian Hydrogen Fundamental Expertise). The research leading to these results has also received funding from the Fund for Scientific Research Flanders (FWO) and innovation program/ERC grant agreement no.818607 (OPTIMA).

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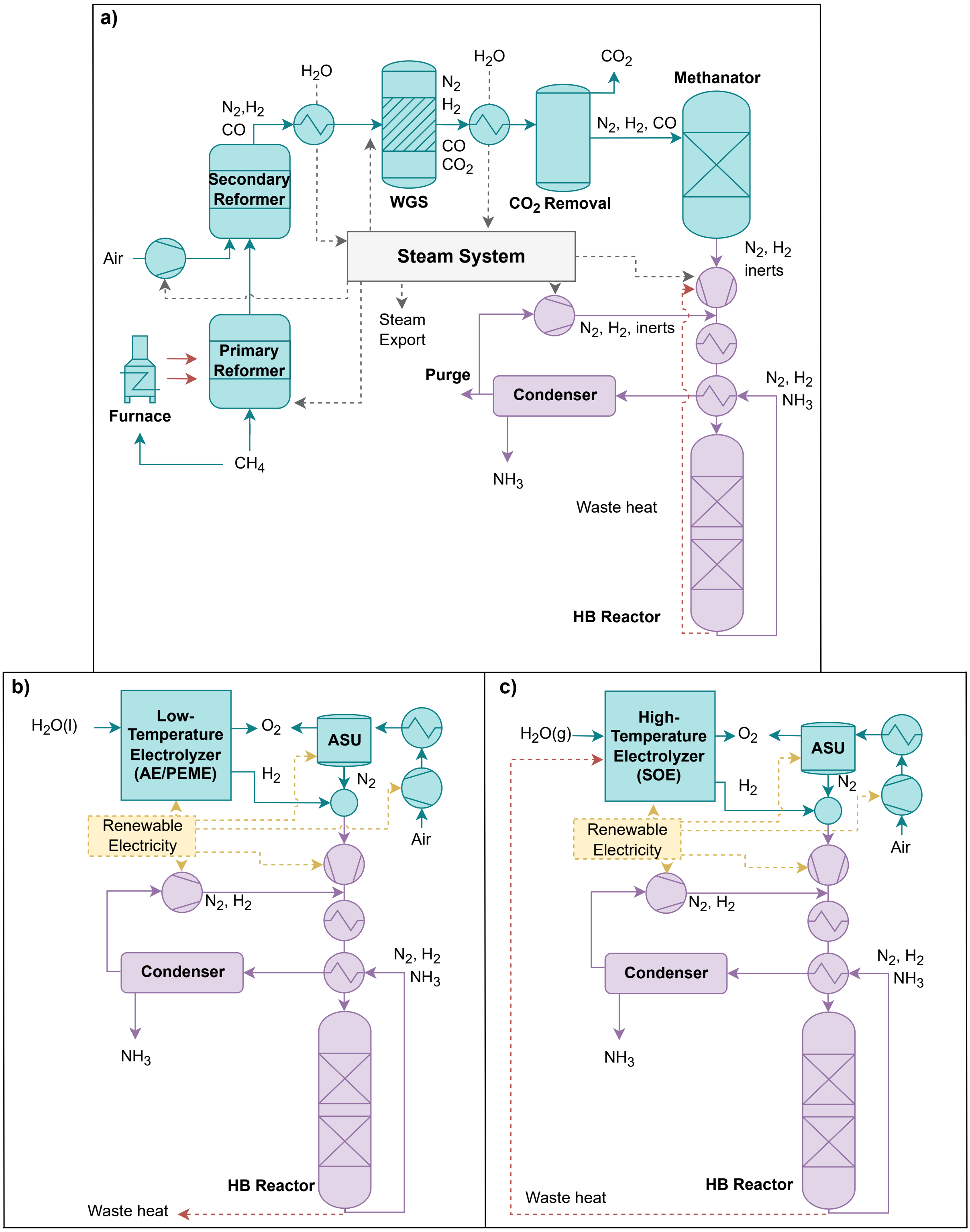

Figure 1. Process diagrams of Scenario 0 (a), 1 (b) and 2 (c). Each has a H2/N2 production unit (turquoise) and a NH_3 production unit (purple). Steam system, renewable electricity and heat recycling are displayed by grey, yellow and red dashed arrows, respectively. Inspired by [4].

Table 1. Operating conditions for each processing step of the 3 scenarios. Data from [4,6,12,18,23,35,36].

Processing step	**Temperature [°C]**	**Pressure [bar]**
Primary reformer	850 – 900	25 – 35
Secondary reformer	900 – 1000	25 – 35
Water Gas Shift (WGS)	200 – 380	10 – 60
CO_2 Removal	-10 – 39	20 – 120
Methanation	250 – 350	25 – 35
Haber-Bosch (HB) Reactor Interstage coolant	350 – 500 50	150 – 300
Condenser	-25	140
Alkaline Electrolyser (AE)	60 – 90	1 – 30
Proton Exchange Membrane Electrolyser (PEME)	50 – 80	10 – 200
Solid Oxide Electrolyser (SOE)	600 - 1000	1 – 25
Air Separation Unit (ASU)	-195 – -170	1 – 10

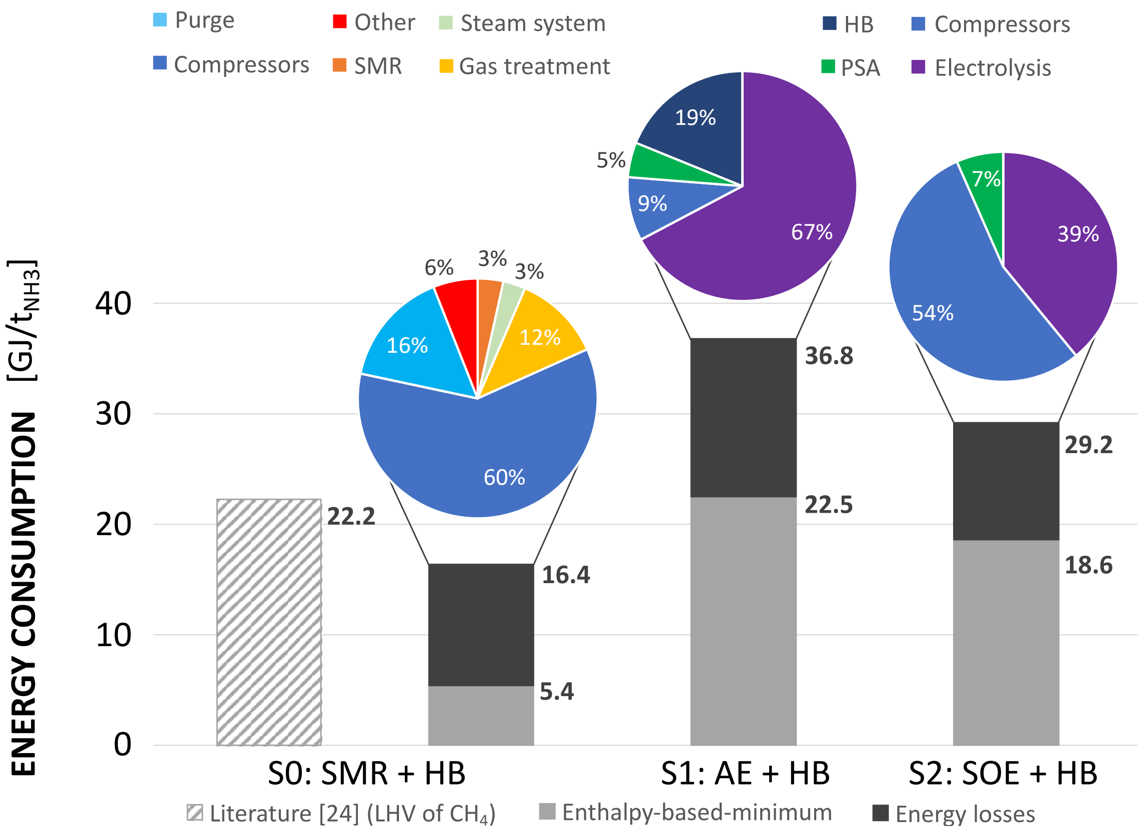

Figure 2. Energy consumption in GJ/tNH3 for Scenario's 0, 1 and 2 (S0, S1, S2). The % color scale refers to the energy losses. Data taken from [4,6,18,23,26].

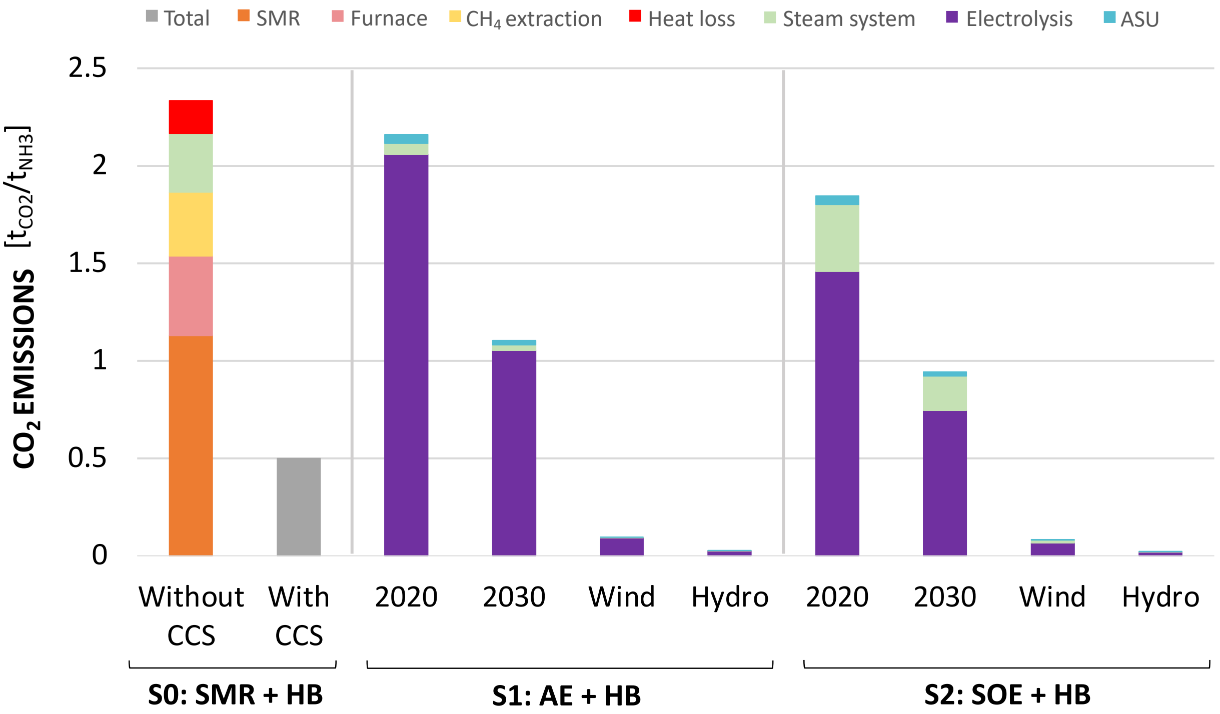

Figure 3. CO2 emissions expressed in tCO2/tNH3 for Scenario's 0, 1 and 2 (S0, S1, S2). Four cases are considered for Scenario 1 and 2: “2020” is based on the present carbon-intensive grid; “2030” is a projection of the current carbon-intensive grid in 2030; “Wind” is based on 100% wind-electricity; and “Hydro” is based on 100% hydro-electricity. Data taken from [4,9,30,32,33]