Flexibility in low-carbon nitrogenous fertilizer industries

A case study for the Dutch fertilizer industry

Technical and economic demand response potential analyses of European low-carbon nitrogenous fertilizer production plants in 2030

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Abstract

Global fertilizer production accounts for 2 – 3% of the total energy consumption of which nitrogenous fertilizer is the vast majority. With natural gas as the dominant source of energy, the fertilizer industry is considered one of the largest greenhouse gas emitting industries. Nowadays, global energy markets are disrupted by Russia's invasion of Ukraine. Thus, reducing natural gas consumption in industries has become of great importance to decrease the EU's dependence on Russian fossil fuels in combination with tackling the climate crisis. In this study, we examine the demand response potential of a European low carbon fertilizer production facility in 2030 by applying a cost minimization linear programming model. First, a consumption and production profile of a fictive European fertilizer plant is estimated based on the current profiles of OCI Nitrogen's and Yara Sluiskil's fertilizer production facilities. Second, the impact on the energy consumption is determined for three decarbonization pathways: Business-as-usual scenario (BAU), Carbon capture and storage scenario (CCS), and a fully electrified Green Ammonia scenario. Third, the technical and economic demand response potentials are estimated through a linear optimization programming model. In the BAU scenario, a fertilizer production facility is expected to consume 34.2 PJ natural gas and 124.5 GWh electricity per year. A CCS system significantly increases the electricity consumption by more than a three-fold, but this is still only a relative energy increase of 3% while 96% of the CO_2 emissions are now captured and stored. In the Green Ammonia Scenario, the total energy requirement increases by approximately 15%. The analysis on future trends of natural gas and carbon permits reports threshold values that show when the Green Ammonia production route is lower in total energy costs compared the BAU and CCS scenario. Concerning the demand response potential, the overall energy cost reduction in the BAU and CCS scenario was close to zero since the share of electricity consumed lower than 3%. Solving the optimization model for the Green Ammonia scenario showed that an economic demand response potential of 3.6% could be achieved with a 16.6% peak shifting potential annually. In this research, the electrolyzer is dimensioned 10% larger than required with an installed capacity of 1.3 GW. The technical and economic demand response potential could potentially be maximized by oversizing the electrolyzer up to a point where the demand response potential is still more profitable than the additional investment and operational costs.

Nomenclature

Table 1. List of abbreviations

Abbreviation	**Definition**
BAT	Best Available Technology
BAU	Business-as-usual
CCS	Carbon capture and storage
DR	Demand response
VRES	Variable Renewable Energy Sources
GHG	Greenhouse gas

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Preface

Fueled by the geopolitical dilemmas regarding the EU's dependence on Russian fossil fuels, I started to examine the impact of natural gas prices on food products in October 2021. Concerning the debate around increasing energy prices in combination with the nitrogen crisis I found out that agricultural practices became a topic of discussion in the Netherlands. This made me eager to gather knowledge on the industrial processes related to fertilizer production. In my personal communication with OCI and Yara International (two of largest nitrogenous fertilizer companies) I found out that soaring natural gas prices have made them decide to shut down their European ammonia production plants. However, there was no available spot at the time to write my thesis at their company. In February 2022, I got in contact with Annika Boldrini, a PhD candidate at Utrecht University and a researcher at the Joint Research Center of the European Commission. She presented me with a possible dissertation topic on flexibility in industries with the fertilizer industry as one of the topics of interest.

When I found out that both OCI Nitrogen and Yara Sluiskil had made their first steps in moving away from natural gas as the dominant energy source for fertilizer production processes I decided to write this thesis at Utrecht University but as a case study for the European fertilizer industry. Since both companies have expressed their interest in green hydrogen in the near future, they are good candidates for a case study on industrial scale flexible fertilizer production.

Throughout the research project, I received weekly supervision from Annika Boldrini. Without her cooperation and guidance it would have been much tougher to conduct the analysis and solve the linear program. In addition, every two weeks I received supervision from Dr. Ir Wina Crijns-Graus who provided me with feedback and guidance on the progression and direction of the research objective.

1. Introduction

1.1 Background

In the Paris Agreement of 2015, 196 parties adopted a legally binding international treaty on climate change which aims at limiting global warming to below 2 ˚C, preferable below 1.5 ˚C, compared to pre-industrial levels (United Nations Climate Change, n.d.). In August 2021, the Intergovernmental Panel on Climate Change published the IPCC Working group I report releasing scientific observed changes in the Earth's climate which state that anthropogenic emissions of greenhouse gasses (GHG) will be responsible for a global changing temperature that is expected to exceed 1.5 ˚C in the next 20 years (IPCC, 2021). To reach this goal, countries must reduce their greenhouse gas emissions to 'net zero' by 2050. However, becoming 'net zero' by 2050 requires a global annual greenhouse gas emissions reduction from 33.9 gigaton of $CO_{2\text{-eq}}$ in 2020 to 0 gigaton of $CO_{2\text{-eq}}$ by 2050 (IEA, 2021b). Since the energy sector is responsible for around 75% of global greenhouse gas emissions, decarbonization of the power sector is considered essential to reach the 1.5 ˚C target (IEA, 2021b). Therefore, clean energy technologies are of high importance to increase the share of renewable energy sources in the fuel mix. However, clean energy technologies often go hand in hand with electrification since renewable energy sources are predominantly converted into electricity, resulting in a 90% required renewables share of the total electricity generation by 2050 to reach the 'net zero emissions target (IEA, 2021b).

Energy-intensive industries are considered the largest greenhouse gas emitters globally, including the production of chemicals, e.g., fertilizers (Worrell et al., 2009). According to Wei, McMillan, & de la Rue du Can (2019), global industrial consumption of final energy accounts for 37% of the total final energy consumption with a heavy reliance on fossil-fuel based combustion for high temperature process heating. As a result, 25% of global greenhouse gas emissions in 2020 were caused by industries (IEA, 2021b), hence, electrified industrial processes have the potential to reduce industry related greenhouse gas emissions substantially (Wei et al., 2019). However, one could imagine that an increased share of renewable energy sources, including intermittent renewable energy sources, coupled with an increased dependence on electricity could cause some endeavors with regards to matching future demand and supply of electricity. As intermittent renewable energy source can threaten the supply reliability of power systems, demand response (DR) is often presented as a demand side management tool for the expansion of renewable energy supply (Bouckaert et al., 2014).

Over the last decades, agricultural activities have intensified as a response to an almost quadrupled human population in the 20th century. The world population is expected to increase by approximately 2 billion people by 2050 (Roell & Zurbriggen, 2020). As a result, global food production must increase accordingly to meet the rising demand by 2050 (Roell & Zurbriggen, 2020)**.** Therefore, we can conclude that the need for synthetic fertilizers is considered quite unlikely to diminish within the next 30 years. Alexandratos & Bruinsma (2012) estimated the global fertilizer consumption in 2050 in million tons of nutrients nitrogen-, phosphorous and potassium-based fertilizers. Their projections state that by 2050 263 million tons of nutrients will be consumed compared to 166 million tonnes in 2005/2007 (Alexandratos & Bruinsma, 2012).

Global fertilizer production accounts for 2 – 3% of the total energy consumption of which nitrogenous fertilizer is the vast majority (European Commission, 2007). In 2018, the global production of fertilizers accounted for 250.9 tonnes of which 58% was produced from nitrogen (Fertilizers Europe, 2019). In EU-28, this share is significant higher, i.e., 74% of the total production of 18.1 million tonnes of fertilizer (Fertilizers Europe, 2019). According to the European Commission (2019), natural gas is generally used to produce nitrogenous fertilizers and approximately 65% of all the natural gas input is used as a feedstock for hydrogen whereas the remaining 35% is burned for high temperature heating steps within the process and electricity generation. As described in more depth in section 2.1, the production process contains several endothermic reactions with high operating temperatures requiring external energy. Most of the energy is required for the conversion of the hydrocarbon feed into hydrogen and the fixation of nitrogen from atmospheric air in the primary and secondary steam methane reforming reactors, both required to produce ammonia (NH_3). Besides ammonia production, also the production of urea ($CO(NH_2)_2$) from ammonia requires a considerable amount of energy. On the other hand, the conversion of ammonia to nitric acid (HNO_3) and the neutralization of ammonia with nitric acid to produce ammonium nitrate (NH_4NO_3) releases energy leading to a net energy gain in the form of heat. This heat is often exported to other endothermic production processes (Ahlgren et al., 2008; Lim et al., 2021).

During the COP 21 in Glasgow, it was established that emissions related to chemical processes must reduce by 20% in 2050 compared to the 2013 levels to meet the targets of the two-degree scenario. In other words, by 2050 ammonia- and nitric acid-related greenhouse gas emission must not exceed 367 Mt $CO_{2\text{-eq}}$/ year and 72 Mt $CO_{2\text{-eq}}$/ year respectively (Lim et al., 2021). Globally, conventional ammonia production alone already accounts for 0.93% of greenhouse gas emissions (Ikäheimo et al., 2018). Average European nitrogenous fertilizer plants have a considerably lower carbon footprint compared to other regions with an average of 1.112 t $CO_{2\text{-eq}}$/ t NH_4NO_3 versus 2.249 t $CO_{2\text{-eq}}$/ t NH_4NO_3 and 2.836 t $CO_{2\text{-eq}}$/ t NH_4NO_3 of average fertilizer plants in North America and China respectively (Hoxha & Christensen, 2018). According to the projections of Lim et al. (2021), global greenhouse gas emissions from the production of ammonia and nitric acid will reach the 900 Mt $CO_{2\text{-eq}}$/ year and 150 Mt $CO_{2\text{-eq}}$/ year by 2050 respectively if ammonia and nitric acid continue to be synthesized through the Haber-Bosch and Ostwald processes under a continuous but constant growing demand. In other words, without switching to alternative ammonia and nitric acid synthesizing methods, the annual emission related to this industry will exceed the targets of two-degree scenario by 245% for ammonia and 208% for nitric acid (Lim et al., 2021).

Since water electrolysis (hydrolysis) is considered the most feasible technology for the conversion of renewable power to chemicals, substituting steam methane reforming reactors for electrochemical synthesis of ammonia from green hydrogen is often seen as a potential decarbonization strategy for nitrogenous fertilizer production (Ikäheimo et al., 2018). The findings of Ikäheimo et al. (2018) show that power-to-ammonia becomes economically competitive if natural gas prices exceed 70 €/MWh, which occurred in the Netherlands in September 2021 (Sönnichsen, 2022a). Nowadays, where natural gas prices are rising due to geopolitical conflicts, reliance on electricity from renewable energy sources could become increasingly important as VRES are considerably lower in price and the supply is far less dependent on geopolitical dilemmas. As a matter of fact, Yara International (a global fertilizer manufacturer) has decided to cut production in two European fertilizer plants as a response to soaring natural gas prices (McDonald & Ram, 2022). Moreover, renewable power-to-ammonia could have a promising demand side management potential for storing renewable power during off-peak electricity demand as a load-shifting tool. Ultimately, electrification of industrial practices inevitably leads to a significant increased electricity demand. In combination with an increasing share of intermittent renewable energy sources in the fuel mix, demand side management tools like DR will become of great importance to match the demand for electricity with the supply from the power-grid.

1.2 Research gap

Existing research papers have identified the theoretical energy requirements of ammonia, nitric acid, ammonium nitrate and urea production. Ikäheimo et al. (2018) estimated that the production of ammonia from nitrogen and renewable hydrogen requires 0.64 MWh_{el}/ t NH_3 including the energy requirements of an air separation unit. Moreover, Wang et al. (2020) simulated a production plant coupling power-based ammonia synthesis with nitric acid production via highly efficient heat integration. This integrated system could lead to 12% total primary energy savings compared to conventional production plants. Furthermore, Ahlgren et al. (2008) determined that producing ammonium nitrate from neutralizing ammonia with nitric acid requires only 25 kWh/ t ammonium nitrate as this exothermic reaction provides enough heat for the water removal step. Lastly, since CO_2 is no longer supplied by renewable ammonia synthesis in the production of urea, Zhang, Wang, Van herle, Maréchal, & Desideri (2021) examined the integration of biomass-fed entrained flow gasifier for the supply CO_2. Their findings show that integrated power- and biomass-to-urea production has a system efficiency of 53% compared to 56% for methane-to-urea (H. Zhang et al., 2021).

These papers lack estimations of the energy consumption patterns of decarbonized nitrogenous fertilizer production on plant scale. Furthermore, previous research of Kelley, Do, & Baldea (2022) examined the DR potential of ammonia plants and concluded that they are promising candidates for DR initiatives because of its high energy intensity and the reliance on a single source demand (Paulus & Borggrefe, 2011). The approach of Kelley et al. (2022) to model an optimal DR scheduling problem of a conventional ammonia plant based on a Hammerstein-Wiener inspired modelling framework has showed a peak-time power consumption reduction between 3.57% - 7.40% in combination with 1.39% - 3.70% operational cost reductions. These findings show that DR initiatives provide promising results with regards to a peak-shifting potential of electricity consumption in industrial fertilizer production plants as well as potential operational costs savings. However, a study estimating the DR potential of a European low-carbon nitrogenous fertilizer plant in 2030 is still missing.

1.3 Research questions

This research paper is structured to answer the following main research question:

"What is the technical and economic demand side response potential of a European low-carbon nitrogenous fertilizer production plant in 2030?"

The following sub-questions help answering the main research question:

1. *"What are the energy consumption profiles of a European nitrogenous fertilizer plant for the production of ammonia, nitric acid, ammonium nitrate and urea and the associated greenhouse gas emissions?"*
2. *"How will the decarbonization pathways alter the energy consumption profile of a conventional nitrogenous fertilizer production plant?"*
3. "How do the decarbonization pathways alter the production costs of nitrogenous fertilizer products?".
4. *"What is the technical demand side response potential of a low-carbon nitrogenous fertilizer production plant?"*
5. *"What is the economical demand side response potential of a low-carbon nitrogenous fertilizer production plant?"*

1.4 Research aim and scope

Since nitrogen is considered the dominant feedstock of fertilizer products in Europe, this research will merely focus on nitrogenous intermediates and fertilizer products, i.e., excluding phosphorous and potassium-based fertilizers. The research will aim at estimating the DR potential of a European low-carbon nitrogenous fertilizer plant in 2030 by identifying the energy consumption profiles of three decarbonization pathways. Additionally, this research will predominantly aim at European nitrogenous fertilizer plants and their projected operation activities in 2030.

2. Theoretical background

2.1 Production process

Chemical fertilizers are produced based on the three major nutrients uptake of crops required for growth and their metabolism: nitrogen, phosphorous and potassium (Alexandratos & Bruinsma, 2012). These three elements can therefore be considered primary nutrients. Calcium, magnesium, sodium, and sulphur are only supplied incidentally and could therefore be considered secondary nutrients. Micro-nutrients like boron, copper, manganese, iron, cobalt, zinc, and molybdenum are occasionally incorporated in the fertilizer product to provide a speciality product (European Commission, 2007). In 2018, the share of European nitrogen-, phosphorous- and potassium-based fertilizers were 74%, 11% and 15%, respectively (Fertilizers Europe, 2019). Alexandratos & Bruinsma (2012) stated that the share of these three fertilizer types is expected to only change marginally until 2050 and could therefore be assumed to remain constant until 2030. 97% of nitrogen-based fertilizers are derived from ammonia and whereas 70% of phosphate-based fertilizers are derived from phosphoric acid (European Commission, 2007). The most important intermediate chemical products used for fertilizer production are NH_3, HNO_3, sulfuric acid (H_2SO_4) and phosphoric acid (H_3PO_4) (European Commission, 2007). Figure 1 provides an overview of the links between the Large Volume Inorganic Chemicals – Ammonia, Acids and Fertilizers. The green area represents the boundaries of this research, where the production of hydrogen is included in the blue area of ammonia production. Ammonia, urea, urea ammonium nitrate, and calcium ammonium nitrate are here considered final products.

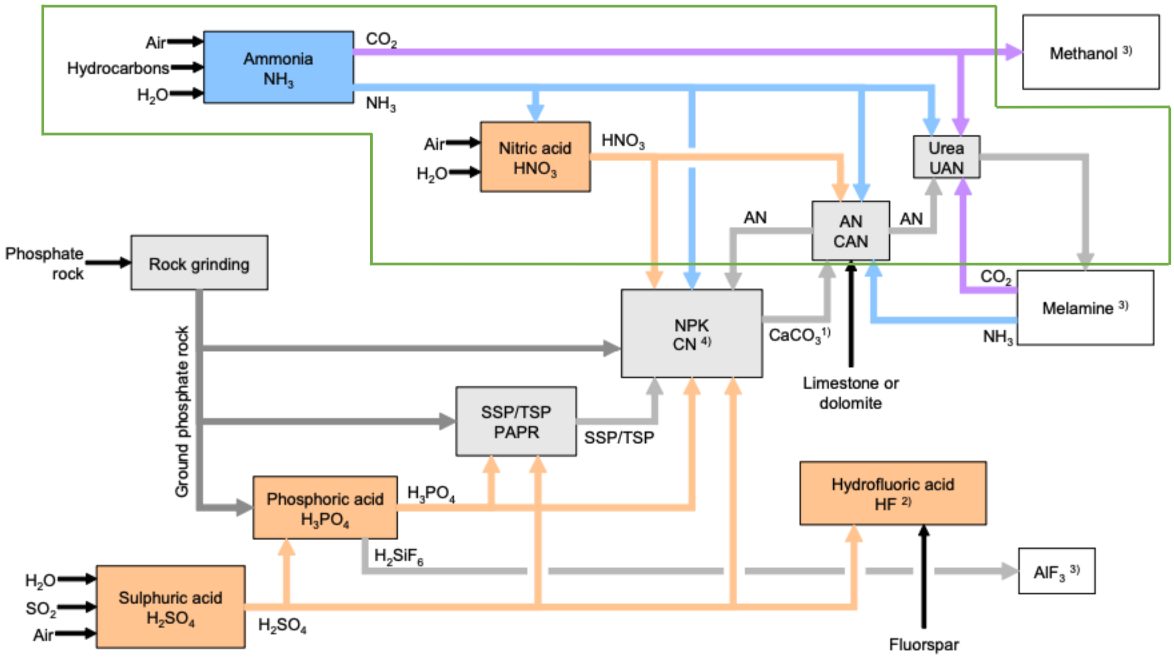


Figure 1. Overview of links between the Large Volume Inorganic Chemicals - Ammonia, Acids and Fertilizers (European Commission, 2007).

Ammonia production (intermediate for fertilizer products)

In 2021, the global production capacity of ammonia amounted to 236.4 million metrics tonnes (Fernández, 2022). Modern commercial size ammonia plants have production capacity of 1000 – 2000 tonnes of ammonia a day (European Commission, 2007). About 20% of the ammonia world-wide is used for various industrial applications while roughly 80% is currently being used as the nitrogen source for several fertilizer products. Ammonia is considered an intermediate product for fertilizer production. The following reaction shows the synthesis of ammonia from nitrogen and hydrogen:

$$N_2 + 3\,H_2 \rightarrow 2\,NH_3 \qquad \Delta H_0 = -46.1\frac{kJ}{mol}$$

The real synthesis that occurs in ammonia plants are far more complex as hydrogen from fossil fuels is derived from natural gas via conventional steam reforming in European and North American plants (Brentrup et al., 2016). In China, hydrogen is often derived from coal via partial oxidation (Brentrup et al., 2016). In conventional European ammonia plants, atmospheric air and natural gas are upgrade to ammonia, as shown as a simplification in the following reaction:

$$N_2 + CH_4 \rightarrow NH_3$$

In 72% of conventional nitrogenous fertilizer production plants ammonia is synthesized from atmospheric air and natural gas (IEA, 2021c). The methane-fed ammonia production route can be divided into two production steps: hydrogen production from methane and ammonia synthesis by the Haber-Bosch route, as schematically visualized in Figure 2. The process that bounds nitrogen with hydrogen to produce ammonia is called the Haber-Bosch process. About 96% of ammonia is produced via the Haber-Bosch nitrogen fixation route (Smith et al., 2020). At first, desulphurization is applied to clean natural gas from sulphur impurities (IEA, 2021c). Following, methane-fed hydrogen production requires primary and secondary steam methane reforming reactors which are considered two high energy intensive reaction steps. In the primary steam methane reforming reactor, desulphurized gas is mixed with steam in the presence of large numbers of catalyst filled tubes at a temperature between 500 ˚C – 600 ˚C (European Commission, 2007). In the convection section, CH_4 and H_2O are converted down to CO and H_2 with a conversion rate of around 60%. In the second steam reforming reactor, compressed air is added to achieve the required nitrogen for the ammonia synthesis step further in the process. After the second steam reforming reactor, the mixture contains 12 – 15% CO (European Commission, 2007). Subsequently, a two-stage water shift reactor maximizes CO conversion to H_2 and CO_2 in the presence of H_2O (Smith et al., 2020). After CO_2 removal, ammonia is synthesized in Haber-Bosch reactor in the presence of an iron-based catalyst (often magnetite or wüstite). Contrarily, the high reaction temperature of the endothermic steam methane reforming reactions produces lots of waste heat at the water-shift reactor that operates at a much lower temperature to minimize carbon monoxide concentrations. Therefore, waste heat is used for creating compression energy needed for the Haber-Bosch loop and the reformer combustion air compressor, as these two are the largest energy intensive processes (Smith et al., 2020)

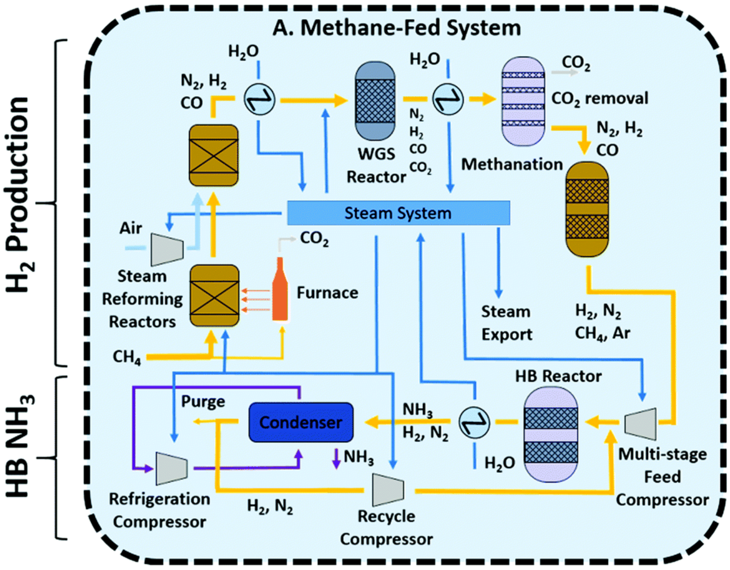


Figure 2. Schematic diagram of a methane-fed Habe- Bosch process system (Smith et al., 2020).

(Calcium) Ammonium nitrate production

Ammonium nitrate is an industrial chemical that is often used in the fertilizer or the explosive industry. One could know ammonium nitrate from the massive explosion in a warehouse in Beirut in 2020. Furthermore, ammonium nitrate is commonly used as a synthetic fertilizer because, when applied in an appropriate ratio, NH_4^+ and NO_3^- could stimulate root development and promote enzyme activity (J. Zhang et al., 2019). The synthesis of ammonium nitrate (NH_4NO_3) requires ammonia and nitric acid, as shown in the following reaction:

$$NH_3 + HNO_3 \rightarrow NH_4HNO_3 + 145.1\ kJ$$

The production of ammonium nitrate requires ammonia (NH_3) and nitric acid (HNO_3). Nitric acid is produced from ammonia and predominantly used for ammonium nitrate production as it neutralizes the final product in combination in the presence of ammonia. The nitric acid synthesis chain is called the Ostwald process which could be divided into three formation reaction; the oxidation of ammonia to form nitric oxide, the oxidation of nitric oxide to nitrogen dioxide and the absorption of nitrogen dioxide in water to form nitric acid and nitric oxide (Cefic, 2013). The oxidation of ammonia is carried out air in the presence of a catalyst, and shown in the following reaction:

$$4NH_3 + 5O_2 \rightarrow 4NO + 6H_2O$$

Subsequently, the formed nitric oxide and water at high pressure are brought to the oxidation tower where nitric oxide gets oxidized again in the presence of additional oxygen to produce NO_2, as shown in the following reaction (Lim et al., 2021):

$$2NO + O_2 \rightarrow 2NO_2$$

Finally, NO_2 goes through the absorption tower where a hydration process leads to the absorption of H_2O to form nitric acid and nitric oxide (Lim et al., 2021). Nitric oxide (NO) is often cycled back for re-oxidation, however, at high pressure and low temperatures, NO tends to decompose to strong greenhouse gasses, such as nitrogen dioxide (NO_2) and nitrous oxide (N_2O) (Cefic, 2013). The following reaction represents the absorption of nitrogen dioxide in water:

$$3NO_2 + H_2O \rightarrow 2HNO_3 + NO$$

Depending on whether the formed nitric acid is in the gas or the liquid phase, the overall heat of the total reaction of nitric acid synthesis from ammonia and oxygen is 369.7 kJ/ mol HNO_3 and 413.8 7 kJ/ mol HNO_3 respectively (Kirova-Yordanova, 2017). Following, ammonium nitrate is produced from nitric acid and ammonia, as shown in the following reaction:

$$NH_3 + HNO_3 \rightarrow NH_4NO_3$$

The production process of ammonium nitrate is comprised of three functional steps, neutralizing, evaporation, and solidification. At first, aqueous nitric acid is neutralized with gaseous ammonia through a highly exothermic reaction producing ammonium nitrate solution (ANS) with enough heat to remove the water in the evaporation step (Ahlgren et al., 2008). After the evaporation step, the process continuous with a mixing step, a prilling or granulation step, and a drying, cooling and conditioning step. In some cases, ammonium nitrate solution is mixed with dolomite, limestone, or calcium carbonate to produce calcium ammonium nitrate which is considered the most applied fertilizer in Western European countries (European Commission, 2007).

Urea and Urea-ammonium nitrate production

Urea is a chemical compound that is produced by protein metabolism and often known as the secreted compound in mammalian urine. Over the past century, urea has become the most dominant solid chemical fertilizer due to its high demand in Asia for flooded rice fields. About 80% of the global urea demand is for fertilizer usage, but urea is also used as a cattle feed supplement because of its high inexpensive nitrogen content (European Commission, 2007). Moreover, urea is considered a low-cost synthetic nitrogen fertilizer with main advantages due to its stability providing simple transportation and storage possibilities. In industrial production of urea, liquid ammonia reacts with gaseous carbon dioxide through the Bosch-Meiser process. The Bosch-Meiser process contains two functional steps; the fast highly exothermic reaction of ammonia and carbon dioxide forming ammonium carbamate (NH_2COONH_4), and the relatively slow and endothermic decomposition of ammonium carbamate into urea ($CO(NH_2)_2$) and water, as shown in the following reaction (Xia et al., 2022):

$$2NH_3 + CO_2 \leftrightarrow NH_2COONH_4 \leftrightarrow CO(NH_2)_2 + H_2O$$

Urea is often prilled or granulated or mixed with ammonium nitrate solution to produce urea ammonium nitrate for storage or distribution. One would argue that the production of urea and urea ammonium nitrate could be considered a carbon dioxide storage application. However, the carbon dioxide within urea is only temporarily stored and released into the air upon spreading.

2.2 CO_2 emissions

Besides their intensive energy consumption profiles, industrial fertilizer production facilities contribute significantly to the global emission of greenhouse gasses. The production of synthetic fertilizers entails several chemical reactions. These chemical reactions produce NO_x, CO_2 and N_2O as by-products. As a matter of fact, the synthesis of ammonia accounts for 1.44% of global $CO_{2\text{-eq}}$ emissions with an average emission factor of 2.86 t $CO_{2\text{-eq}}$ / t NH_3 (Soloveichik, 2019). This is mainly caused by the fact that the Haber-Bosch process is considered one of the largest global natural gas consumers, hence, one of the largest greenhouse gas emitters (Smith et al., 2020). Nonetheless, Yara Sluiskil published in their sustainability report that almost 90% of their N_2O emission are abated using catalytic cleaning technologies (Batool & Wetzels, 2019). Although the nitrogenous fertilizer industry aims at implementing various mitigation technologies to reduce its environmental footprint, for instance by using catalysts that mitigate nitrous oxide emissions, most efficient plants still produce 1.8 t $CO_{2\text{-eq}}$ / t NH_3 (IEA, 2021c).

2.3 Decarbonization pathways

Over the last couple of decades, decarbonization pathways have slowly been implemented at several stages in the synthetic chemical fertilizer industry. As mentioned earlier, fertilizer production plants of Yara Sluiskil and OCI Nitrogen implemented catalytic cleansing technologies that abates 90% of all N_2O emissions. As a result, greenhouse gas abatement technologies should aim at reducing CO_2 emitting production processes. Since ammonia production is reliant on natural gas as a feedstock and a fuel, decarbonizing the fertilizer industry is most effective when natural gas could be substituted by green hydrogen as a feedstock for the steam reforming process and the electrification of the processes for heat and power (Batool & Wetzels, 2019). Smith et al. (2020) state that the ammonia synthesis loop can only become an almost carbon-free production process when 1) the hydrogen supply and the steam reforming reactors are decoupled from methane, 2) condensing steam turbines and compressors are electrically driven, and 3) ammonia separation techniques are improved requiring lower operating pressure to reduce the total electricity requirements of the process, as schematically visualized in Figure 3.

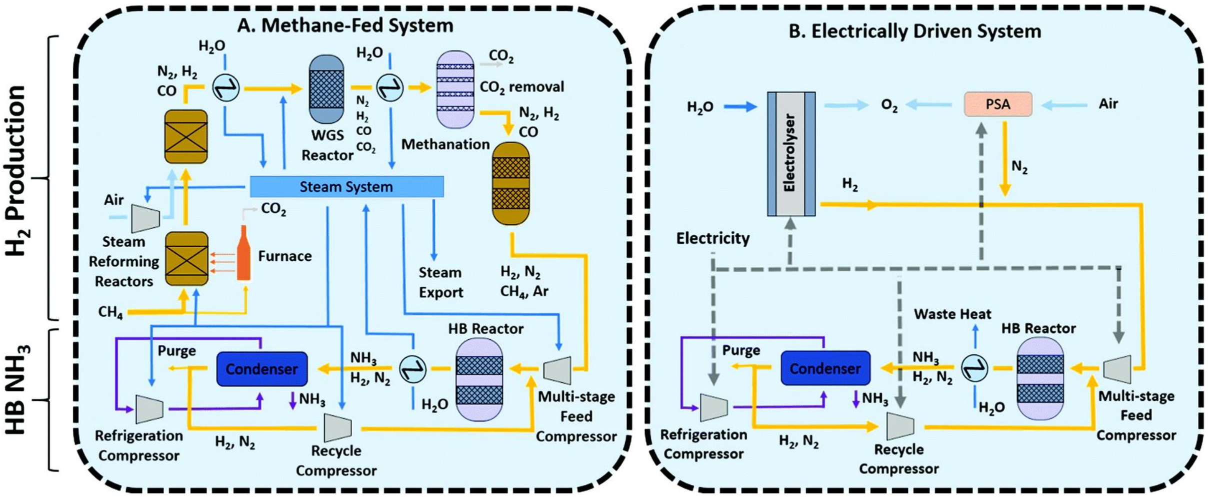


Figure 3. Schematic diagram of a conventional methane-fed Haber Bosch process system and an electrically driven ammonia production system (Smith et al., 2020).

An electrolyzer can produce H_2 and O_2 from H_2O by passing an electrical current through an electrolyte in between an anode and a cathode (Batool & Wetzels, 2019). This electrolyzer has the potential to operate on renewable electricity supply producing green hydrogen. A green hydrogen fed ammonia loop could improve its energy efficiency by 50% (Humphreys et al., 2021). Moreover, the findings of Smith et al. 2020) estimated that a green hydrogen fed ammonia loop could potentially reduce the 1.67 t CO_2/ t NH_3 of methane fed ammonia production to 0.38 – 0.53 t CO_2/ t NH_3. An electrolyzer produces H_2 and O_2 according to the following reaction:

$$2H_2O \rightarrow 2H_2 + O_2, \qquad \Delta H_0 = 571.8\,\frac{kJ}{mol}$$

2.4 Demand side management

Decarbonization strategies for nitrogenous fertilizer production that aim at switching to green hydrogen and electrification of the production processes inevitably requires the implementation of variable renewable energy sources. Due to the intermittency of renewable energy source, electricity fed ammonia, ammonium nitrate and urea syntheses go hand in hand with changes in consumers pattern of industrial production facilities. This paradigm shift, where instantaneous consumption patterns move towards a more flexible consumption pattern, requires strategic demand side management. The latter could be achieved by demand side management tools to minimize curtailment. The minimization of curtailment is often achieved by shifting the energy demand via price optimization during peak and off-pike electricity demand (Finn & Fitzpatrick, 2014).

DR encompasses electricity price, incentive payments or resource availability as demand-side management tools to changes electricity consumption patterns of customers (López et al., 2015; McPherson & Stoll, 2020). The findings of McPherson & Stoll (2020) have shown that the importance of DR tools increases for higher renewable energy penetration as they increase the operational flexibility of the power system, Figure 4. The flexible load potential is often assessed by two methods, an aggregated method where changes in demand are assessed according to market conditions, and the decomposition method where the potential of flexible load is assessed by determining flexible and inflexible component within the system. The latter will be used in this research paper as it allows for decomposition of electricity consumption in multiple processes.

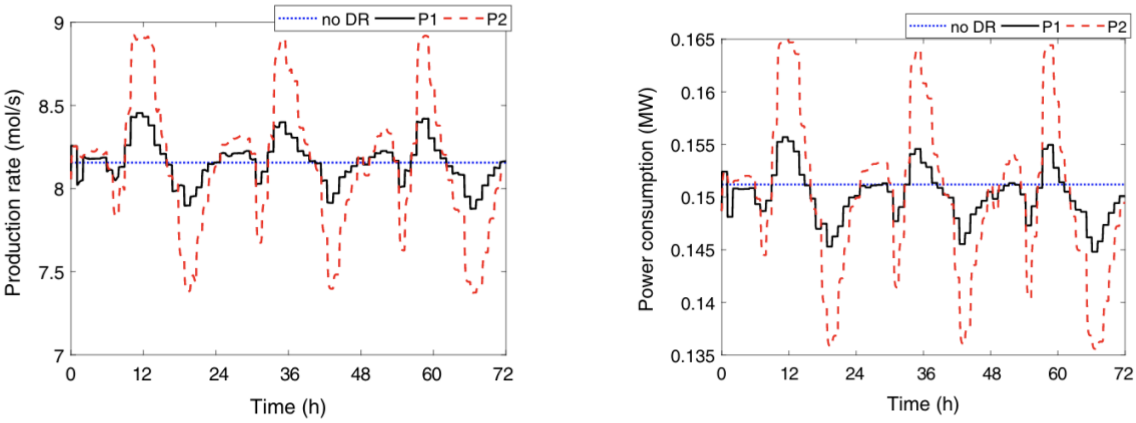


Figure 4. Ammonia production rate operating under DR conditions (Kelley et al., 2022).

The DR potential is often expressed in total operation costs reduction and peak-price hour power consumption (MW). The definition of DR consists of multiple categories: theoretical, technical, economic, and achievable potential. At first, the theoretical potential could be defined as the absolute maximum potential and comprises all facilities and devices of the consumer unrestricted electricity demand (Dranka & Ferreira, 2019). Secondly, as derived from the theoretical potential, the technical potential is smaller than the theoretical potential as it includes technical restrictions, for instance, installed capacity, annual load hours, maximum production speed, total production output, shifting time, and the number and duration of interventions (Dranka & Ferreira, 2019). Lastly, as derived from the technical potential, the economic potential also includes economic restrictions (Dranka & Ferreira, 2019).

3. Research Framework

A research framework is designed to structure the research as the sub-research questions will be answered sequentially because the answer to one sub-question provides the input data for the following one, as visualized in Figure 5. The research can be divided into two sequential phases in which a different quantitative analysis method will be used. At first, the energy demand profile and CO_2 emissions of a fictive European nitrogenous fertilizer production plant are estimated based on existing European fertilizer production faculties. Figure 5 presents all fertilizer production facilities in the Netherlands. For this research, only nitrogenous fertilizer plants are taken into consideration.

Figure 5. Map of fertilizer production plants in Europe (Fertilizers Europe, 2018).

The energy consumption profiles of OCI Nitrogen's and Yara Sluikil's integrated nitrogenous production facilities are identified and estimated through desk-research, public company data, and short interviews with both companies. OCI Nitrogen is selected since it is considered one of the market leaders in fertilizer products in Europe. As part of OCI N.V., OCI Nitrogen is a nitrogen fertilizer and melamine producer located in Geleen, the Netherlands (Chemlot, n.d.). Their nine interconnected plants produce anhydrous ammonia, calcium ammonium nitrate, urea ammonium nitrate and melamine. The nitrates production facility is considered the second largest producer in the Europe (OCI N.V., n.d.). Moreover, OCI joined the largest hydrogen project of Europe called NorthH2. In their announcement, OCI stated that they will be willing to purchase 1 gigawatt green hydrogen the moment it becomes available (Sluijters, 2022). Potentially, the NorthH2 consortium will be located at the Eemshaven and fed with renewable energy generated from wind energy in the North Sea. The NorthH2 has the ambition to produce 4-gigawatt green hydrogen by 2030 of which one-fourth will be available for the OCI plants (Sluijters, 2022).

Furthermore, Yara Sluiskil is one the production facilities of Yara International located along the canal between Gent and Terneuzen. This site has Europe's largest installed ammonia and nitrate fertilizer production facilities containing two ammonia plants, four CO_2 plants, two nitric acid plants, two urea plants and two nitrate granulation plants (Yara Internatioal, n.d.). Two years ago, Yara and Ørstad (world's leading offshore wind developer) joined forces to develop a green hydrogen project. The aim of the project was to build a 100 MW wind power electrolyzer plant by 2024 – 2025 (Yara International, 2020). A 100 MW electrolyzer could potentially substitute 10% of the capacity of one of their grey ammonia plants. Ultimately, both companies are considered first movers in creating a sustainable future for fertilizer products.

The research steps followed in the research framework are visualized in Figure 6. Because no standard nitrogenous fertilizer production facility exists due to various intermediate and final products, the energy consumption profile of a fictive European plant is determined by adjusting the OCI Nitrogen and Yara Sluiskil production facilities based on future projections of energy efficiency in existing literature, step 1. Subsequently, the energy demand profiles of a fictive low-carbon nitrogenous fertilizer plant will be estimated for the business-as-usual scenario and two decarbonization pathways (i.e., carbon capture and storage, and electrification), step 2. In step 3, the production costs of the three pathways are estimated based on future projections of energy prices and CO_2 permits. Lastly, solving the optimization model of the linear problem provides us the technical and economic DR potential of a low-carbon fertilizer plant will be determined based on multi-objective optimization modelling, step 4, 5 and 6.

The following assumptions are made:

- The analysis will not include transportation costs and emissions of the feedstocks nor the final products and maintenance of the fertilizer plant.
- The production capacity of the fictive European plant will remain the same in 2030 as the year from which the data is gathered

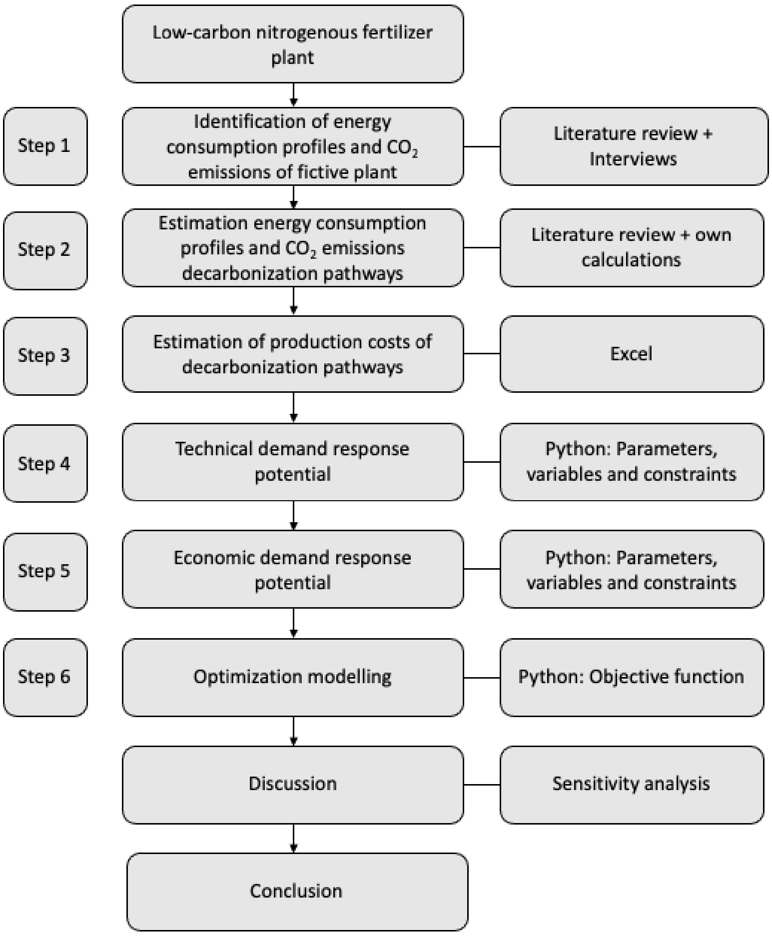


Figure 6. Research framework.

4. Estimation of energy demand profiles and CO_2 emissions of a conventional fertilizer production plant

In this section the hourly energy demand profile and CO_2 emissions of a fictive European fertilizer production plant is determined to answer the first sub-research question “What are the energy consumption profiles of a European nitrogenous fertilizer plant for the production of ammonia, nitric acid, ammonium nitrate and urea and the associated greenhouse gas emissions?”. The energy demand profiles of the production of ammonia, nitric acid, ammonium nitrate and urea are estimated based on the existing energy consumption patterns of either the OCI Nitrogen plant or the Yara Sluiskil plant from published company data. Based on annual sustainability reports of OCI Nitrogen and Yara Sluiskil, annual nitrogen-fertilizer related CO_2 emissions are determined for ammonia, nitric acid, ammonium nitrate and urea production. Since both OCI Nitrogen or Yara Sluiskil were not willing to share more detailed data on the energy consumption profiles of their existing fertilizer production plants, the energy demand profile of the fictive European fertilizer plant is predominantly determined based on the provided data of *Decarbonization Option for the Dutch Fertilizer Industry* report of Batool & Wetzels (2019) and the *Perspective Europe 2030 - Technology options for CO_2-emission reduction of hydrogen feedstock in ammonia production* report of Ausfelder et al. (2022). For all production processes, the maximum production capacity, storage capacity, and the maximum production speed are determined in section 5. Furthermore, calculations of the production of intermediates and final products are based on Table 2, providing the world average feedstock and input values for each product (Kool et al., 2012).

Table 2. The amount of feedstock needed to produce 1 ton of product (Kool et al., 2012).

Product	Input	Value	Unit
Nitric Acid	Ammonia	0.27	t/ t product
Urea	Ammonia	0.57	t/ t product
	CO_2	0.73	t/ t product
Ammonium nitrate	Ammonia	0.22	t/ t product
	Nitric aicid	0.81	t/ t product
Urea ammonium nitrate	Urea	0.35	t/ t product
	Ammonium nitrate	0.46	t/ t product
Calcium ammonium nitrate	Dolomite	0.24	t/ t product
	Ammonium nitrate	0.76	t/ t product

4.1 Ammonia synthesis

The energy intensity of the full production process of ammonia is usually expressed on a gross basis or a net basis. Expressing the energy intensity on a net basis means that there is accounted for the generation of energy by deducting excess steam produced throughout the production process. In this paper, the energy intensity of ammonia synthesis is expressed on a net basis. In 2020, the global average energy requirement for ammonia production was estimated to be 41 GJ per tonne (IEA, 2021c). This is large number is mainly due to the high energy intensive production route of ammonia from coal gasification which is used in 26% of the ammonia produced globally (IEA, 2021c). Producing hydrogen through a methane-based steam reforming process requires a significant amount of energy due to the endothermic hydrocarbon feed conversion reaction, however, it is considered relatively energy efficient compared to coal gasification.

In 2020, the total energy requirement of best available technology (BAT) of ammonia synthesis from natural gas and atmospheric air ranges is estimated to be 28 GJ per tonne NH_3 (IEA, 2021c), as shown in Table 3. The lower heating value of ammonia equals 18.6 GJ per tonne NH_3 which implies that if all heat in the process will be recovered, the thermodynamic minimum of ammonia synthesis would require 18.6 GJ per tonne NH_3 (Cefic, 2013). However, in conventional ammonia synthesis plants additional energy is required for the reformation reaction resulting in theoretical minimum of 23 GJ per tonne NH_3. The report of Cefic (2013) estimated that new grey ammonia plants could reach an energy demand of 28 GJ/ t NH_3 in 2020, 27 GJ/ t NH_3 by 2030 and 26 GJ/ t NH_3 by 2050, as shown in Table 3. This is in line with the 2020 BAT published by the IEA (2021c). However, the projections of Ausfelder et al. (2022) estimated that new grey ammonia plants would require 7.7 MWh/ t NH_3 or 27.9 GJ/ t NH_3 by 2030 which is slightly higher.

Table 3. Net energy consumption profiles for ammonia synthesis.

4.77	Net energy consumption		[GJ / t NH3]
Best available technology	Fuel	Natural gas	11.1
		Electricity	0.3
		Steam	-4.8
	Feedstock	Natural gas	21.0
	Total		27.6
OCI AFA-2	Total		31.7
OCI AFA-3	Total		31.7
Yara C	Total		30.5
Yara D	Total		30.5
Yara E	Total		30
Expected plant 2030	Total		27
Expected plant 2050	Total		26

OCI Nitrogen

At OCI Nitrogen, anhydrous ammonia is produced in two plants (AFA-2 and AFA-3) with a combined capacity of 1184 kt per year. With approximately 8000 operating hours a year, these two plants produce approximately 2962 tonne ammonia per day resulting in 1081 kt ammonia per year. Table 4 shows that the production of 1 tonne anhydrous ammonia requires 14.6 GJ and 20.7 GJ of natural gas as a fuel and feedstock respectively (Batool & Wetzels, 2019). In other words, the production of ammonia is estimated to require 35.3 GJ natural gas and 0.3 GJ electricity per tonne NH_3. However, due to the interconnected plants, waste heat produced during ammonia synthesis is exported to other production plants. Therefore, the total net energy consumption could be defined as total consumption – export, i.e., 31.7 GJ / tonne NH_3. Per tonne of NH_3 produced, 2.0 tonnes of $CO_{2\text{-eq}}$ are generated compared to 1.8 tonnes of CO_2 per tonne NH_3 in the BAT steam methane reformer (Cefic, 2013).

Table 4. Estimates of technical parameters of two OCI Ammonia plants (Batool & Wetzels, 2019).

	Ammonia plant (AFA-2 and AFA-3)
Capacity [kt/year]	1184
Operating hours [h]	8000
Production [kt product / year]	1081
Input of natural gas (fuel) [GJ/t product]	14.6
Input of natural gas (feedstock) [GJ/ t product]	20.7
Input of natural gas total [GJ/t product]	35.3
Net input of steam [GJ/ t product]	-3.9
Net input electricity [GJ/ t product]	0.3
Total energy input [GJ/ t product]	31.7
CO_2 emissions (combustion) [t CO_2/ t product]	0.7

CO_2 emissions (high purity CO2) [t CO_2/ t product]	1.3
CO_2 emissions (total) [t CO_2/ t product]	2.0

Yara Sluiskil

At Yara Sluiskil, ammonia is produced in three plants with a combined capacity of 1.8 million tonnes per year. With approximately 8000 operating hours annually, these plants produce 1.6 million tonnes of ammonia a year with an average daily production of 4.6 kt. Table 5 shows that plant C till plant E have an increasing installed capacity and a decreasing total net energy input because of their construction year with plant C being the oldest facility and plant E being the newest. Based on the weighted average of the installed capacity the rightmost column represents the average input and output of the total production of three plants combined. Table 5 shows the input of natural gas as a feedstock is similar for both OCI Nitrogen and Yara Sluiskil facilities. Considering a similar net input of steam and electricity of -3.9 GJ and 0.3 GJ respectively, Yara's ammonia plants are slightly more energy efficient with a total net energy input of 30.3 GJ/ t NH_3 (Batool & Wetzels, 2019). However, this is still 2.5 GJ/ t NH_3 more energy intensive compared to the BAT. Furthermore, in terms of greenhouse gas abatement techniques, with 1.9 t CO_2/ t NH_3 Yara Sluiskil has been able to bring their $CO_{2\text{-eq}}$ emissions produced closer to the BAT of 1.8 tonnes of CO_2 per tonne NH_3 compared to 2.0 t CO_2/ t NH_3 for OCI Nitrogen(Cefic, 2013).

Table 5. Estimates of technical parameters of three Yara Sluiskil Ammonia plants (Batool & Wetzels, 2019).

	Ammonia plant C	Ammonia plant D	Ammonia plant E	Ammonia plants total
Capacity [kt/year]	459	639	731	1829
Operating hours [h]	8000	8000	8000	8000
Production [kt product / year]	410	584	668	1662
Input of natural gas (fuel) [GJ/t product]	13.4	13.4	12.9	13.2
Input of natural gas (feedstock) [GJ/ t product]	20.7	20.7	20.7	20.7
Input of natural gas total [GJ/t product]	34.1	34.1	33.6	33.9
Net input of steam [GJ/ t product]	-3.9	-3.9	-3.9	-3.9
Net input electricity [GJ/ t product]	0.3	0.3	0.3	0.3
Total energy input [GJ/ t product]	30.5	30.5	30.0	30.3
CO_2 emissions (combustion) [t CO_2/ t product]	0.6	0.6	0.6	0.6
CO_2 emissions (high purity CO2) [t CO_2/ t product]	1.3	1.3	1.3	1.3
CO_2 emissions (total) [t CO_2/ t product]	1.9	1.9	1.9	1.9

4.2 Nitric acid synthesis

Nitric acid is considered both an intermediate and a final product in the fertilizer production industry. Reactions taking place in nitric acid plants are highly exothermic. As a matter of fact, the formation of nitric acid from ammonia theoretically releases 6.3 GJ/ t HNO_3 (Wiesenberger, 2001). Therefore, nitric acid production plants also produce steam or mechanical energy. However, since a significant amount of energy is required for gas compressors and water cooling throughout the process, the total energy export is reduced when residual thermal energy could be converted to electrical power in a steam turbine (European Commission, 2007). Considering the energy benchmark system, 43% of 83 nitric acid plants had an overall energy export by turning a power deficit into a power surplus through energy recovery techniques (Lako, 2009). This benchmark had a range of -1.8 GJ/ t HNO_3 to +3.8 GJ/ t HNO_3 of total energy export (Lako, 2009). Therefore, in the report of Batool & Wetzels (2019) they assumed that the net input of steam to produce nitric acid could be considered 0 GJ / t nitric acid.

Table 6 shows that for the synthesis of 1 tonne nitric acid approximately 0.27 tonne of ammonia is needed in both OCI Nitrogen's and Yara's nitric acid plants. Moreover, no external steam or natural gas is required for the production process due to the highly exothermic reactions as described earlier. However, a total of 0.1 GJ net input of electricity is required which is predominantly used for compressions (European Commission, 2007). Notably, rather than CO_2 emissions caused by the combustion of natural gas or the conversion of hydrocarbon, the production of nitric acid leads to N_2O emissions. OCI Nitrogen and Yara Sluiskil aimed at abating their N_2O emissions by implementing catalytic cleansing technologies which have led to 90% overall N_2O emissions reduction (Tezel & Helmer, 2020). Nevertheless, their average N_2O emissions of 0.6 kg N_2O/ t HNO_3 are still on the highest part of the BAT spectrum of 0.2 – 0.6 kg N_2O/ t HNO_3 (Batool & Wetzels, 2019). This could be explained by the fact that the lower spectrum of the BAT is achieved by new nitric acid production plants whereas the BAT of existing plants ranges up to 1.85 kg N_2O/ t HNO_3 (Overgaag M. et al., 2009).

Table 6. Estimates of technical parameters of Yara Sluiskil's and OCI Nitrogen's nitric acid plants.

	Nitric acid plant OCI Nitrogen	Nitric acid plant Yara Sluiskil
Capacity [kt/year]	965	1500
Operating hours [h]	8000	8000
Production [kt product / year]	881	1370
Average daily production [t]	2414	3753
Input of ammonia [t NH3/ t product]	0.27	0.27
Input ammonia [kt]	238	370
Input of natural gas [GJ/t product]	0	0
Net input of steam [GJ/ t product]	0	0
Net input electricity [GJ/ t product]	0.1	0.1
CO2 emissions (total) [tCO2/ t product]	0	0
N_2O emission [kg N_2O / t product]	0.6	0.6
N_2O emission [t N_2O]	502	780
N_2O emission [Mt $CO_{2\text{-eq}}$]	0.1	0.2
GHG emission [Mt $CO_{2\text{-eq}}$]	0.1	0.2

4.3 (Calcium) Ammonium nitrate production

Ammonium nitrate is produced from ammonia and nitric acid. This neutralization reaction is exothermic resulting in high release of reaction heat which is used to evaporate the water present in the diluted nitric acid. However, some additional steam is required as the heat of reaction is not enough to evaporate all the remaining water (Kirova-Yordanova, 2017). Kirova-Yordanova (2017) estimated that the total consumption of steam in ammonium nitrate plants varies between 10 and 150 kg moderate pressure steam per tonne NH_4NO_3. In conventional plants, export steam generated in ammonia and nitric acid plants is used for ammonium nitrate production. Export steam generated in ammonia and nitric acid plants is substantially more than required for ammonium nitrate synthesis. As a matter of fact, when ammonia will be synthesized via a more sustainable route substituting its reliance on methane, the total export steam generated will reduce significantly. Nonetheless, export steam only generated in a conventional nitric acid plant can still meet the needs of the ammonium nitrate plant (Kirova-Yordanova, 2017). When calcium ammonium nitrate is produced, dolomite is added in the mixing step before the prilling tower or granulator to produce Western Europe's most applied fertilizer product (European Commission, 2007). The production of 1 tonne of calcium ammonium nitrate requires 0.24 tonne dolomite and 0.76 tonne ammonium nitrate (Kool et al., 2012).

Assuming OCI Nitrogen and Yara Sluiskil both produce ammonium nitrate based on the stoichiometric ratio of Table 2, the production of 1 tonne ammonium nitrate via the conventional methane-fed steam reforming route results in a total consumption of 13.9 and 13.4 GJ of methane per tonne ammonium nitrate respectively for OCI Nitrogen's and Yara's AN plant.

4.4 Urea (ammonium nitrate) production

Urea is synthesized from liquid ammonia and gaseous CO_2 through the Bosch-Meiser process. All CO_2 captured as a by-product in the ammonia plant will not be enough to feed the urea plant because per two moles NH_3 produced only $\frac{7}{8}$ CO_2 is formed (Kirova-Yordanova, 2017). To convert all ammonia into urea, the remaining required CO_2 should be added. The synthesis of ammonium carbamate is fast and exothermic; however, the reaction heat is released at low temperatures leading to insufficient steam generation. Following, the dehydration of carbamate to urea and water is slightly endothermic with an unfavourable equilibrium up to 65% (Kirova-Yordanova, 2017). Although the overall reaction from ammonia and CO_2 to urea is exothermic, it is significant less efficient than ammonium nitrate synthesis. Since urea plants are usually integrated in the ammonia synthesis plant, the energy requirement of a stand-alone urea plant is hard to estimate. The findings of Kirova-Yordanova (2017) show that the overall production of 1 tonne of urea requires 850 – 1000 kg moderate pressure steam (2.2 GJ) and 0.3 GJ of electricity.

Table 7. Estimates of technical parameters of Yara Sluiskil's and OCI Nitrogen's urea plants.

	Urea plant OCI Nitrogen	Urea plant Yara Sluiskil
Capacity [kt/year]	525	1300
Operating hours [h]	8000	8000
Production [kt product / year]	479	1187
Average daily production [t]	1312	3252
Input of ammonia [t NH3/ t product]	0.57	0.57
Input ammonia [kt]	273	677
Input of CO_2 [t CO_2/ t product]	0.73	0.73
Input of CO_2 [Mt]	0.4	0.9
Input of natural gas total [GJ/t product]	0	0
Net input of steam [GJ/ t product]	2.2	2.2
Net input electricity [GJ/ t product]	0.3	0.3
CO_2 emissions (total) [t CO_2/ t product]	0	0

Table 7 represents the estimations of the production and consumption details of OCI Nitrogen's and Yara's urea plants. Notably, the installed capacity of Yara's urea plant is almost 2.5 times as large as OCI's urea plant. As presented earlier in Table 2, the production of 1 tonne urea requires 0.27 tonne ammonia and 0.73 tonne CO_2 (Kool et al., 2012). The estimated numbers in Table 7 are in accordance with the paper of Kirova-Yordanova (2017) who stated that despite an overall exothermic reaction, the production of urea requires the import of steam and a net input of electricity. For both OCI and Yara, the production of 1 tonne of urea requires 2.2 GJ of steam and 0.3 GJ electricity.

Following, dissolved concentrated urea and liquid ammonium nitrate are heated and mixed in either a continuous or batch process to produce a liquid urea-ammonium nitrate fertilizer. This mixing step does not lead to any form of greenhouse gas emissions nor waste products (European Commission, 2007). The production of 1 tonne of urea-ammonium nitrate requires 0.35 tonne urea and 0.46 tonne ammonium nitrate (Kool et al., 2012).

4.5 Production facility OCI Nitrogen in Geleen

In this section, the integrated nitrogen fertilizer production facility of OCI Nitrogen in Geleen is observed to get a clear overview of the daily energy consumption pattern and fertilizer production. Considering an estimated annual production of 1081 kt ammonia and the assumption of 8000 load hours per year, on average 2962 tonnes of ammonia are produced per day. Based on the provided estimated production capacity of OCI's ammonia, nitric acid, urea, ammonium nitrate and calcium ammonium nitrate plants of Batool & Wetzels (2019), a material flow diagram is created as shown in Figure 7. Figure 7 represents the energy consumption, $CO_{2\text{-eq}}$ emissions and material flow of an average daily consumption based on the following assumptions:

1. The fertilizer production faculties run for 8000 hours annually resulting in approximately 31.7 days per year of maintenance period.
2. The input of materials is based on Table 2.
3. Urea-ammonium nitrate production cannot be maximized when calcium ammonia nitrate production runs at maximum speed and vice versa. Since the capacity of the urea-ammonium nitrate is significantly smaller than the calcium ammonium nitrate, i.e., half in size, there is assumed that urea-ammonium nitrate production is maximized, and calcium ammonium nitrate is produced at a speed where the remaining ammonium nitrate is consumed considering negligible nitric acid export.
4. Hourly production is calculated by dividing the annual production by the number of annual load hours. This is done by the assumption that maintenance is done one period per year resulting in a plant turn-around period of 31.7 consecutive days.
5. The nitric acid plant produces enough process heat due to the highly exothermic reaction to provide its evaporation and compression steps with the required energy input.
6. The ammonia plant and the nitric acid plant produce enough reaction heat to supply the ammonium nitrate plant with its additional required steam input, as described in section 4.3 (Kirova-Yordanova, 2017).

Table 8. Hourly production details of OCI's integrated fertilizer production.

Compound	Production speed	Unit
Ammonia	135	t / hour
Nitric acid	110	t / hour
Ammonium nitrate	136	t / hour
Urea	60	t / hour
UAN	83	t / hour
CAN	128	t / hour
CO_2 emissions	270	t CO_2/ hour
NO_2 emissions	66	kg NO_2 / hour

Table 9. Hourly consumption details of OCI's integrated fertilizer production.

Fuel	Consumption speed	Unit
Natural gas	4.77	TJ / hour
Electricity	69.5	GJ/ hour

Integrated fertilizer production plants of OCI Nitrogen at Geleen

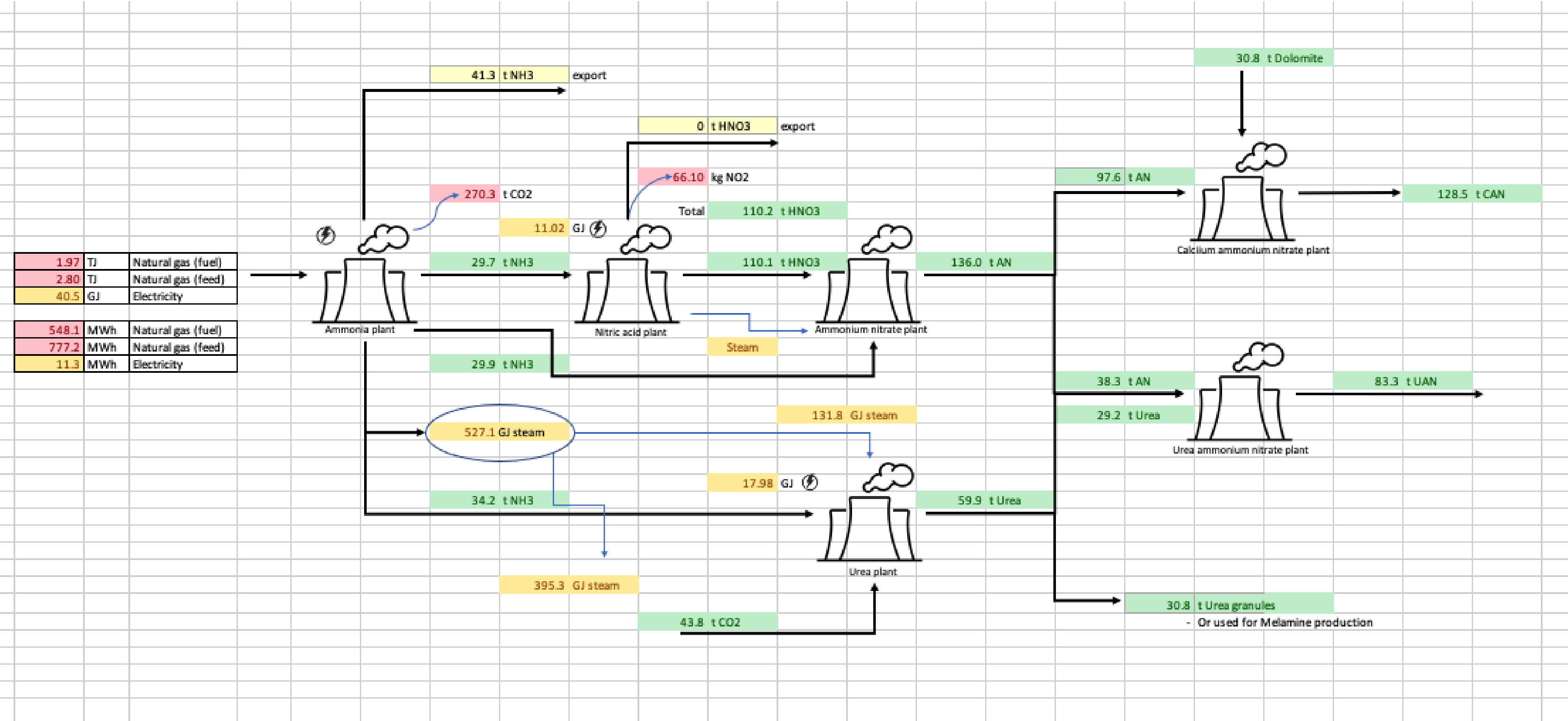


Figure 7. OCI's integrated fertilizer plants' hourly consumption and production profile.

4.6 Production facility Yara Sluiskil

Following, the plants of Yara Sluiskil are observed to create an energy and material flow diagram of the integrated nitrogen fertilizer production facility. This provides a clear overview of the daily energy consumption pattern and fertilizer production. Concerning 8000 load hours per year, ammonia plant C, D and E combined produce 1662 kt ammonia per year, 4553 tonnes ammonia daily and 208 tonnes hourly. The material flow diagram is based on the provided estimated production capacity of Yara's ammonia, nitric acid, urea, and urea ammonium nitrate plants of Batool & Wetzels (2019). Figure 8 shows the energy consumption, $CO_{2\text{-eq}}$ emissions and material flow of an average hourly production day based on the following assumptions:

1. Assumptions 1, 2, 4 – 6 of section 4.5
2. The estimated nitric acid production is much larger than the amount of nitric acid required to produce the estimated urea ammonium nitrate production. Therefore, there is assumed that no nitric acid is exported and that the remaining nitric acid is consumed in the production of ammonium nitrate granules.
3. The annual ammonia export is calculated based on the remaining ammonia after consumption as intermediate product.

Table 10. Hourly production details of YARAI's integrated fertilizer production

Compound	Production speed	Unit
Ammonia	208	t / hour
Nitric acid	171	t / hour
Ammonium nitrate	211	t / hour
Urea	148	t / hour
UAN	104	t / hour
AN granules	163	t / hour
CO_2 emissions	395	t CO_2/ hour
NO_2 emissions	103	kg NO_2 / hour

Table 11. Hourly consumption details of YARA's integrated fertilizer production

Energy source	Consumption speed	Unit
Natural gas	7.3	TJ / hour
Electricity	124	GJ/ hour

Integrated fertilizer production plants of Yara at Sluiskil

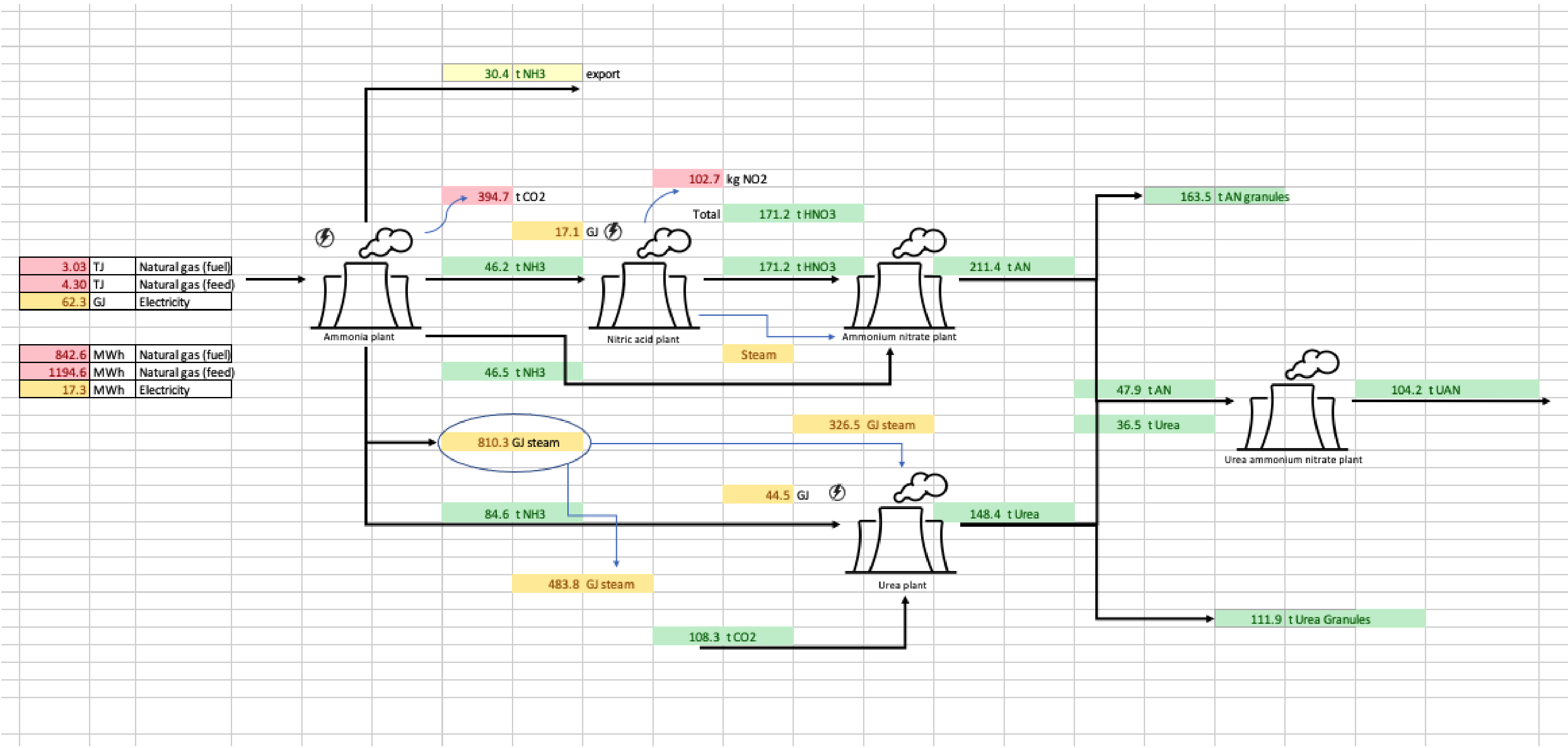


Figure 8. Yara's integrated fertilizer plants' hourly consumption and production profile.

4.7 Conclusion

Previous sections provide a clear overview of how the current fertilizer production facilities of OCI Nitrogen and Yara Sluiskil operate. The hourly energy requirements of the fertilizer plants are presented in Table 12. Conventional fertilizer plants merely run on natural gas with relatively low electricity input. OCI Nitrogen and Yara Sluiskil are two different production facilities with both similar and different final products. Nonetheless, their energy consumption profile expressed in ton product produced are quite similar as most of the energy is consumed during the production of ammonia. Furthermore, no external energy is required to produce ammonium nitrate, urea ammonium nitrate or calcium ammonium nitrate.

Table 12. Hourly energy requirement of the fertilizer plants.

Hourly energy requirement	OCI Nitrogen	Yara Sluiskil
Ammonia plant (natural gas) [GW]	1.3	2.0
Ammonia plant (electricity [MW]	11.3	17.3
Nitric acid plant (electricity) [MW]	3.1	4.8
Urea plant (electricity) [MW]	5.0	12.4

Table 13 shows the fertilizer production related greenhouse gas emissions of OCI Nitrogen and Yara Sluiskil. The ammonia plant is the cause of CO_2 emissions whereas the NO_2 emissions are related to the nitric acid plant. OCI Nitrogen and Yara Sluiskil have both invested in cleaning technologies reducing their NO_2 emissions. This has led to negligible NO_2 emissions and CO_2 emissions quite close to the current Best Available Technology of 1.8 t CO_2 / t ammonia.

Table 13. Hourly total greenhouse gas emissions.

Hourly greenhouse gas emissions	OCI Nitrogen	Yara Sluiskil
CO_2 emissions [t CO_2/ t ammonia]	2.0	1.9
CO_2 emissions [t CO_2/ per hour]	270	395
NO_2 emissions [kg NO_2 / t nitric acid]	0.6	0.6
NO_2 emissions [kg NO_2 / per hour]	66	103

Although the figures in upper tables slightly differ between the two production facilities, both the energy consumption profile and the greenhouse gas emissions per tonne of product could be considered somewhat similar for both companies. Therefore, only one of the production facilities is used to determine the energy consumption profile including the associated CO_2 emissions of a fictive European nitrogenous fertilizer plant in 2030. The mass flow of intermediate products of OCI Nitrogen's facility are determined based on fewer assumption compared to the Yara Sluiskil facility. Inevitably, fewer assumptions lead to less uncertainties, hence, the OCI production facility is used in the following sections.

5 Estimation of energy demand profiles and CO_2 emissions of decarbonization pathways

In this section the hourly energy demand profile and CO_2 emissions of a decarbonized European fertilizer production plant is determined for the following three scenarios to answer the second sub-research question *“How will the decarbonization pathways alter the energy consumption profile of a conventional nitrogenous fertilizer production plant?”.*

- BAU-scenario (grey ammonia): based on the Best Available Technology (BAT) of a European natural gas fed nitrogenous fertilizer plant by 2030. Decarbonization scenarios are analyzed in comparison to this BAU-scenario
- Carbon capture and storage scenario (blue ammonia): Ammonia production plants produce almost pure CO_2 which is now captured during the CO_2 removal stage after the two-stage water gas shift reactor. In addition, CO_2 emissions during combustion of natural gas should also be captured, however, with a lower capture rate compared to the pure CO_2 stream. Compression of the captured CO_2 requires energy which should be done by electric compressor
- Electrical driven production plant (green ammonia): Ammonia loop fed by green hydrogen from an electrolyzer and electric compressors replacing condensing steam turbine compressors in all plants.

For all three scenarios, the estimated production and consumption profile of OCI Nitrogen’s integrated production facility in previous section is used as a foundation to determine the future energy consumption profile of nitrogenous fertilizer production plant. The energy demand requirements of a fictive European plant where hypothetically a decarbonization strategy is implemented is now estimated by altering the production and consumption profile of OCI Nitrogen’s integrated fertilizer production facility based on projections examined in existing literature. The existing literature provides theoretical data on how energy efficiencies will change by implementing the above-mentioned alternative strategies by 2030.

5.1 Business-as-usual scenario (grey ammonia)

In the business-as-usual scenario, the energy consumption profile of an integrated nitrogen fertilizer production facility is be determined based on the projections of the development of the BAT of ammonia, nitric acid, and urea production. As aforementioned, the report of Cefic (2013) made a projection for the energy efficiency improvement of new grey ammonia plants. Their extrapolation of previous trends estimated that a new grey ammonia plant would require 27 GJ to produce 1 tonne of NH_3 by 2030 by reducing natural gas consumption as a fuel and improving the integrated heat system. Their projection assumes that the consumption of natural gas as a feedstock would remain constant until 2030, which is in line with the future projections of Ausfelder et al. (2022). Therefore, the natural gas consumption of the fictive plant is based on the OCI Nitrogen facility with the BAT prognosis on natural gas input parameters and steam production of IEA (2021c), and electricity input parameters of Ausfelder et al. (2022). Table 14 represent the new energy consumption profile of a fictive ammonia plant by 2030. Figure 8 shows the energy consumption, $CO_{2\text{-eq}}$ emissions and material flow of an average hourly production day based on the BAU-scenario conditions.

Table 14. Net energy consumption profiles of a new ammonia plant by 2030.

Ammonia plant	Net energy consumption		GJ / t NH3
New ammonia plant 2030	Fuel	Natural gas	10.9
		Electricity	0.2
		Steam	-4.8
	Feedstock	Natural gas	20.7
	Total		27

Ammonia-related greenhouse gas emissions will reduce in the couple decades due to the implementation of CO_2-abatement technologies. According to the findings of Ausfelder et al. (2022), the current Best Available Technology of 1.8 t CO_2/ t NH_3 will reduce by 0.1 t CO_2/ t NH_3 per decade leading to an emission factor of 1.7 t CO_2/ t NH_3 by 2030 in the business-as-usual scenario. Changes in the future demand for nitrogenous fertilizers are beyond the scope of this research. Therefore, the projection of the future energy consumption profile and greenhouse gas emissions of an integrated fertilizer production facility will not be adjusted to any changes in future demand and supply. In other words, the production data of OCI Nitrogen are assumed to remain constant until 2030.

In the BAU-scenario, the hourly production speed of all fertilizer intermediates and final products equals the production speed of OCI's fertilizer production facility estimated in section 4. The OCI production facility is currently less energy efficient than the BAT. Moreover, compared to the OCI facility, a fictive European production plant in 2030 should at least reduce its energy requirements in the ammonia plant from 31.7 GJ to 27 GJ/ t NH_3 and the associated CO_2 emission from 2.0 t CO_2 to 1.7 t CO_2 / t NH_3. The hourly production and consumption details of a fictive fertilizer production facility in the BAU-Scenario by 2030 are presented in Table 15 and Table 16 respectively. Figure 9 presents an hourly overview of such a profile in BAU Scenario by 2030.

Table 15. Hourly production details of a fictive integrated fertilizer production facility in BAU-scenario by 2030

Compound	**Production speed**	**Unit**
Ammonia	135	t / hour
Nitric acid	110	t / hour
Ammonium nitrate	136	t / hour
Urea	60	t / hour
UAN	83	t / hour
CAN	128	t / hour
CO_2 emissions	216	t CO_2/ hour
NO_2 emissions	66	kg NO_2 / hour

Table 16. Hourly consumption details of a fictive integrated fertilizer production facility in BAU-scenario by 2030

Energy source	**Consumption speed**	**Unit**
Natural gas	4.27	TJ / hour
Electricity	56.0	GJ/ hour

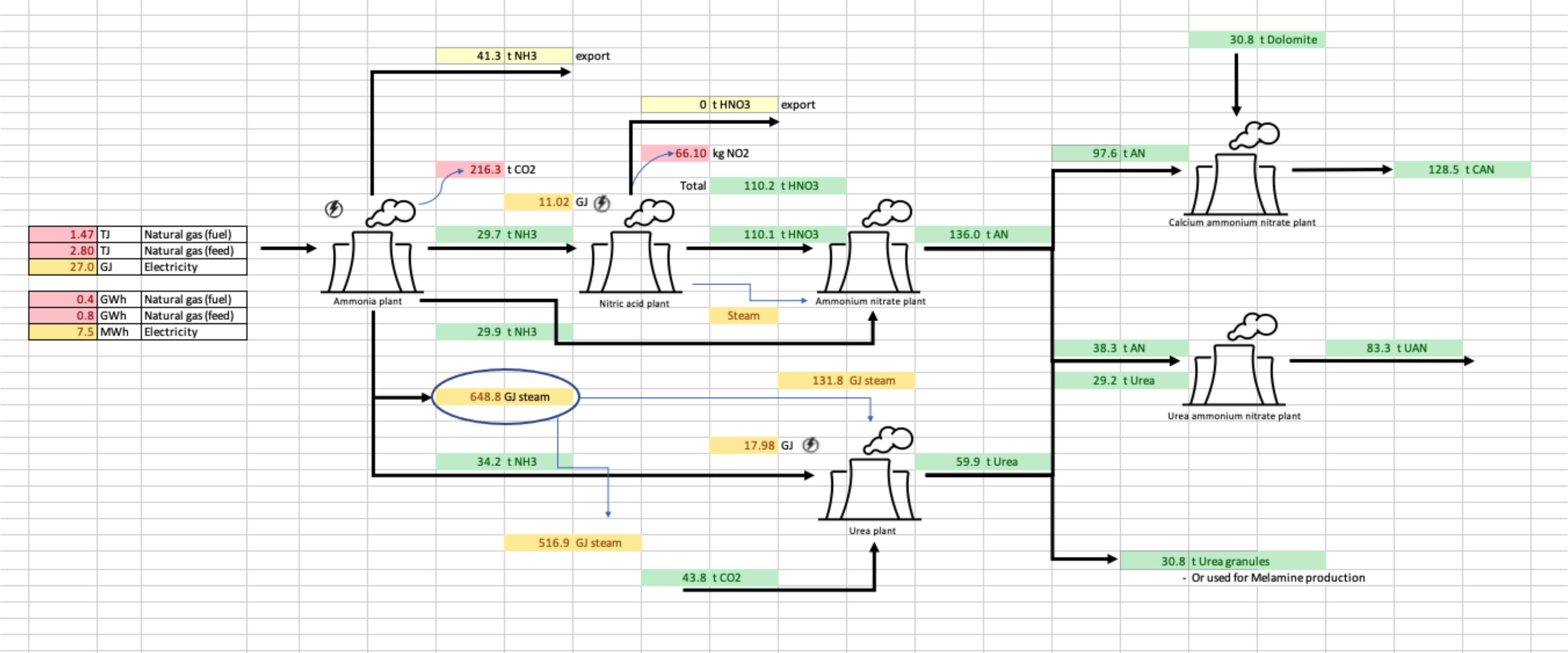


Figure 9. Hourly consumption and production profile of an integrated fertilizer plant in the BAU-scenario by 2030.

5.2 Carbon capture and storage

Depending on the ammonia production route and the hydrogen input, ammonia knows multiple classifications. At first, the production of ammonia through the conventional steam methane reforming route is called grey ammonia synthesized from grey hydrogen. Secondly, when ammonia is exclusively produced form renewable energy sources, it is called green ammonia. Lastly, producing ammonia from fossil-based hydrogen through for instance the steam methane reforming pathway combined with carbon dioxide capture systems results in blue ammonia production. Several studies have showed that fossil-based ammonia production through the steam-methane reforming route will remain the dominant technology, despite its negative environmental impact, due to low cost, availability of resources and technological advancement (Chisalita et al., 2020). Therefore, carbon capture and storage can play an increasing role in low-carbon hydrogen production. Moreover, carbon capture and storage is economically more viable than then coupling of renewable energy sources with electrolysis-based hydrogen production in terms of investment costs (Chisalita et al., 2020). However, the findings of Navas-Anguita et al. (2021) show that blue hydrogen would only emerge as a dominant option in short-to-medium term (2020 – 2030) whereas green hydrogen will take over in the medium-to-long term (2030-2050) as they expected that hydrogen production from fossil-fuels will be banned within the next decades, i.e., between 2030 and 2040. Although it will take a long time for green hydrogen to emerge as a cost-effective alternative, it could occur earlier than Navas-Anguita et al. (2021) projected due to the current trend of rising natural gas prices.

In this decarbonization pathway, a CCS system will be retrofitted in the projected 2030 BAT steam methane reforming route. In the CCS retrofit, both diluted and concentrated CO_2 will be captured and stored. The capture rate of a CCS system depends on the origin from which the CO_2 is produced, i.e., combustion of natural gas or reforming natural gas to flue gas. Existing CO_2 capture systems have an efficiency of 100% for high purity CO_2 gas (Batool & Wetzels, 2019). With amine-based capture technologies, an optimum capture rate between 85% and 90% can be achieved for CO_2 gas produced as a by-product during methane combustion, as shown in Table 17 (IEA, 2021c).

Table 17. Energy requirements for carbon capture and compression in the blue carbon scenario.

	Batool and Wetzels (2019)			IEA (2021c)
Capturing technology	High purity CO_2	CO_2 combustion (2020)	CO_2 combustion (2030)	Combined (2020)
Capture rate	100%	85%	85%	94%
Heat requirements [GJ/ t CO_2 captured]	0	3.2	0	1.7
Electricity requirements [GJ/ t CO_2 captured]	0.4	0.48	1.13	0.7

Separation and compression of CO_2 leads to an increase of the energy requirements when retrofitting carbon capture and storage in an existing ammonia production plant. According to the ammonia roadmap of the IEA (2021c), besides heat input capturing CO_2 would require 0.7 GJ of electricity per tonne ammonia produced. In an isolated ammonia plant the energy requirement to produce 1 tonne ammonia would increase with 0.7 GJ electricity and 1.7 GJ of steam (IEA, 2021c). Compared to the BAT in 2030, the production of ammonia from natural gas with CSS would require 29.4 GJ/ t NH_3 according to the data of IEA (2021c). However, by 2030 a CCS system merely consumes electricity and will not interfere with the existing integrated steam system as all heat and power systems are being electrified. The energy requirement of a CCS system is based on the findings of Batool & Wetzels (2019) as presented in Table 17. Table 17 shows that a CCS system will consume 0.4 GJ of electricity per ton high purity CO_2 captured and 1.13 GJ of electricity per ton CO_2 captured from combustion by 2030.

Table 18. Detailed overview of ammonia-related CO_2 emissions.

Technical parameters	OCI Nitrogen's ammonia plant 2020	Fictive ammonia plant 2030
Production [kt product / year]	1081	1081
Average daily production [t]	2962	2962
CO_2 emissions (total) [t CO_2 / t product]	2	1.7
CO_2 emissions (total) [Mt CO_2] /year]	2.16	1.84
CO_2 emissions (high purity CO_2) [t CO_2/ t product]	1.3	1.3
CO_2 emissions (high purity CO_2) [Mt CO_2/ year]	1.41	1.41
CO_2 emissions (combustion) [t CO_2/ t product]	0.7	0.4
CO_2 emissions (combustion) [kt CO_2 / year]	757	432

Following, the fertilizer production, energy consumption and greenhouse gas emission profile of a fictive European fertilizer production facility is estimated for 2030. The impact of a CCS system is calculated based on the energy requirement of a CCS system shown in Table 17 and the ammonia related CO_2 emissions presented in Table 18. Table 18 also shows how far the current OCI Nitrogen facility is away from the projected BAT by 2030.

The following assumptions are made in the Blue Ammonia scenario:

- The carbon capture and storage system is retrofitted in the BAU scenario resulting in equal energy requirements to produce (intermediate) fertilizer products
- Capturing and storing one tonne high purity CO_2 and one tonne CO_2 from combustion requires 0.4 GJ and 1.13 GJ respectively.

The estimated fertilizer production, energy consumption and greenhouse gas emission profile of a fictive European fertilizer production facility is presented in Table 19 and Table 20. Figure 10 presents an hourly overview of such a profile in Blue Ammonia Scenario by 2030.

Table 19. Hourly production details of a fictive integrated fertilizer production facility in Blue Ammonia scenario by 2030

Compound	Production speed	Unit
Ammonia	135	t / hour
Nitric acid	110	t / hour
Ammonium nitrate	136	t / hour
Urea	60	t / hour
UAN	83	t / hour
CAN	128	t / hour
CO_2 emissions	6.1	t CO_2/ hour
NO_2 emissions	66.1	kg NO_2 / hour

Table 20. Hourly consumption details of a fictive integrated fertilizer production facility in Blue Ammonia scenario by 2030

Energy source	Consumption speed	Unit
Natural gas	4.27	TJ / hour
Electricity	178.24	GJ/ hour

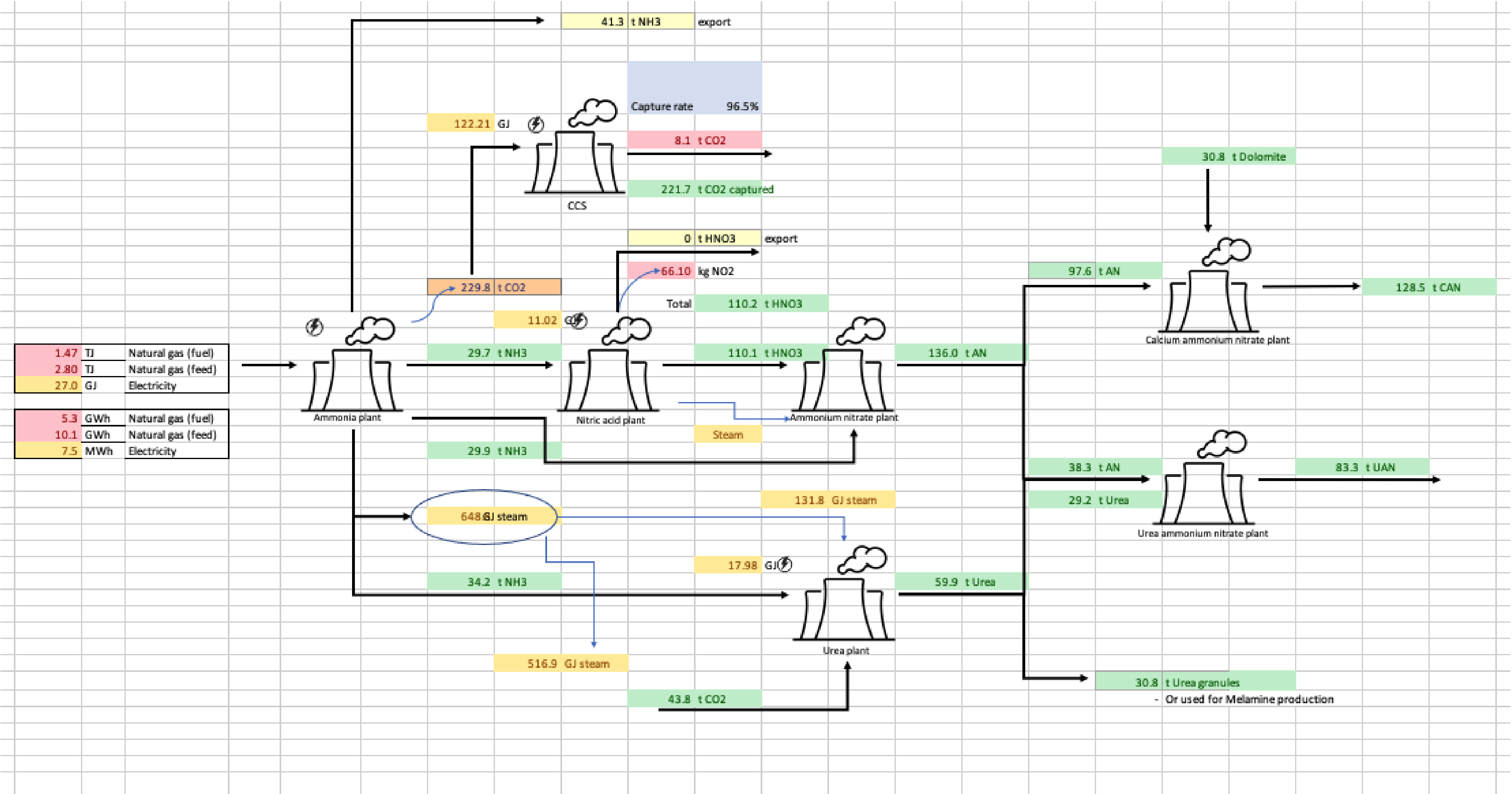


Figure 10. Hourly consumption and production profile of an integrated fertilizer plant in the CCS scenario by 2030.

5.3 Electrified synthesis of green hydrogen fed ammonia, nitric acid and urea using electricity for heat and power

Since methane-fed ammonia production is considered the most energy intensive and polluting step in the nitrogenous fertilizer industry, multiple alternative ammonia synthesis methods have been examined to create a carbon free ammonia synthesis production route. Electrolysis-based ammonia production, for instance, has become increasingly popular due to its potential of consuming renewable electricity. According to the IEA, total electric ammonia production is expected to exceed 3 Mt capacity by 2030 (IEA, 2021c). Moreover, electrolysis-based ammonia production is considered one of the promising decarbonization routes to reduce the consumption of fossil fuels and GHG emissions of the fertilizer industry to meet the 'net zero' targets by 2050. (IEA, 2021b).

5.3.1 Green ammonia

In this research, green ammonia is defined as the production of ammonia through electrolysis-based hydrogen production which is predominantly depending on renewable energy sources. For the 2050, it is assumable that the fuel mix contains 100% energy sources which is needed meet the 'net zero' target by 2050 (IEA, 2021b). However, 100% renewable energy sources in the fuel-mix by 2030 is rather ambitious. Therefore, this research considers only direct CO_2 emissions, thus, electricity fed ammonia production is considered a green ammonia production route. Electrolysis-based hydrogen production essentially means that an electric current is used to electrochemically split water (H_2O) into hydrogen (H_2) and oxygen (O_2) (Ausfelder et al., 2022). There are various types of electrolyzers yet developed or that are still under development. All different types exist of the same fundamental principles of an electrolyzer being two electrodes (cathode and anode), a membrane and an electrolyte (the solution). There are three processes to electrochemically split water: alkaline electrolysis, proton exchange membrane, and solid oxide electrolyzer (Ausfelder et al., 2022). Alkaline electrolyzers are commonly used in chemical industries because of their relatively inexpensive catalysts with a longer durability (IEA, 2021c). A proton exchange membrane, also known as a polymer electrolyte membrane, is a slightly newer design which has proven to be more adaptable to changes in capacity requirements. Lastly, the solid oxide electrolyzer, when deployed at scale, has the potential for relatively higher conversion efficiencies and the ability to operate as a fuel cell (the reversed reaction of electrolysis), however, this design is still under development (IEA, 2021c).

Different from steam methane reforming reactors where methane reacts with oxygen from atmospheric air leading to pure nitrogen for the Haber-Bosch synthesis, electrolysis-based ammonia production requires an additional air separation unit (ASU) to extract pure nitrogen from air (Ausfelder et al., 2022; IEA, 2021c). In addition, a standalone Haber-Bosch synthesis unit is also needed since the ammonia production plant is not an integrated production process anymore when applying electrolysis-based hydrogen production. Both the Haber-Bosch synthesis unit and the air separation unit have the potential to be electricity powered creating a possibility to completely electrify the ammonia production process. According to IEA (2021c), a fully electrified green hydrogen-fed ammonia production plant would require 36 GJ of electricity per tonne ammonia produced. This estimation assumes that 95% of the electricity is used for hydrogen production and 5% used as power for both the air separation unit and the Haber-Bosch synthesis, which is approximately 34.2 and 1.8 GJ respectively. Ausfelder et al. (2022) estimated that the synthesis of green ammonia in fully electrified production plant would require 10.9 MWh_{el} per tonne ammonia produced, i.e., 39.2 GJ of electricity. They state that 8.5 MWh_{el} (30.6 GJ) is needed for the electrolytic hydrogen production and the remaining 2.4 MWh_{el} (8.6 GJ) for the air separation and Haber-Bosch synthesis units. 30.6 GJ per tonne ammonia is in line with the findings of who estimated that the production of 1 kg H_2 requires 47 kWh (Ikäheimo et al., 2018), compared to 53 kWh/ kg H_2 estimated by Batool & Wetzels (2019). The energy requirements for the air separation unit and the Haber-Bosch process are slightly varying in the existing literature. The IEA (2021c) estimated that this would require 1.8 GJ/ t NH_3, whereas

Ikäheimo et al. (2018) state that the compressors in the Haber-Bosch process already requires 0.64 MWh_{el}/ t NH_3 (2,3 GJ/ t NH_3), without taking the ASU into account. Batool & Wetzels (2019) estimated that the total electricity demand for the electricity-fed production of 1 tonne ammonia in either an OCI Nitrogen plant or a Yara plant is around 40.2 GJ/ t NH_3 of which 6.2 GJ for the compression and separation. The estimated energy requirement of an electrolyzer-based ammonia production plant that is used in this paper is represented in Table 21.

Table 21. Electricity demand for electrolyzer-based ammonia production.

Technical parameters	Fictive electrolyzer-based ammonia plant 2030
Operating hours [h]	8000
Production of ammonia [kt product / year]	1081
Hydrogen required [t/ t ammonia]	0.178
Hydrogen required [kt/ year]	192
Electricity demand for electrolysis [kWh/ kg hydrogen]	47
Electricity demand for electrolysis [kWh/ kg ammonia]	8.4
Electricity demand for electrolysis [GJ/ t ammonia]	30.6
Electricity for compressors and air separation unit [MWh/ t ammonia]	1.73
Electricity for compressors and air separation unit [GJ/ t ammonia]	6.2
Electricity demand (total) [GJ/ t ammonia]	36.8
Capacity of electrolyzers [GW]	1.5

Table 21 shows that the electrification of the conventional ammonia production plant of OCI Nitrogen with an estimated annual production of 1.1 Mt ammonia require an electrolyzer with a capacity of 1.5 GW (Batool & Wetzels, 2019). According to the IEA (2021a), the global installed electrolyzer capacity in 2020 accounted for 0.3 GW and is expected to increase up to 17 GW by 2026. Nowadays, large projects range from 10 – 100 MW which is more than one order of magnitude lower than the electrolyzer capacity required for the OCI Nitrogen site.

5.3.2 Electrified fertilizer production facility.

In this section, an electrified nitrogen fertilizer production facility is simulated to get a clear overview of the daily energy consumption pattern and fertilizer production. Considering an estimated annual production of 1081 kt ammonia and the assumption of 8000 load hours per year, on average, 2962 tonnes of ammonia are produced per day. With 8000 load hours annually, a material flow diagram of an electrified nitrogen production facility is created as shown in Figure 11. Figure 11 represents the energy consumption, $CO_{2\text{-eq}}$ emissions and material flow of an average daily consumption based on the following assumptions:

1. The fertilizer production faculties run for 8000 hours annually resulting in 760 hours per year of maintenance period. The annual maintenance is planned in one period resulting in a plant turn-around period of 31.7 days.
2. The energy consumption profile of the fictive plant is based on the production profile of OCI Nitrogen’s integrated fertilizer facility
3. The input of materials is based on Table 2 and Table 21.
4. The annual maintenance is planned in one period resulting in a plant turn-around period of 31.7 days.
5. As described in section 4.3, when ammonia is produced via a fully electrified synthesis route, the nitric acid plant still produces enough reaction heat to provide both its own plant and the ammonium nitrate plant with its required energy input for evaporation and compression.

6. Since the energy requirements of an isolated urea plant are hard to estimated due to its integration in the ammonia synthesis plant and the 2.2 GJ of steam required to produce 1 t NH_3 is not released by in an electrified ammonia plant, the 2.2 GJ of steam are assumed to be substituted by 2.2 GJ of electricity resulting in 2.5 GJ total electricity needed for 1 tonne urea (Batool & Wetzels, 2019).

The estimated fertilizer production, energy consumption and greenhouse gas emission profile of a fictive green ammonia fed European fertilizer production facility is presented in Table 22 and Table 23. Figure 11 presents an overview of the hourly profile of a fertilizer production facility in Green Ammonia Scenario by 2030.

Table 22. Hourly production details of a fictive integrated fertilizer production facility in green hydrogen scenario by 2030

Compound	Production speed	Unit
Hydrogen	24	t / hour
Ammonia	135	t / hour
Nitric acid	110	t / hour
Ammonium nitrate	136	t / hour
Urea	60	t / hour
UAN	83	t / hour
CAN	128	t / hour
CO_2 emissions	0	t CO_2/ hour
NO_2 emissions	66	kg NO_2 / hour

Table 23. Hourly consumption details of a fictive integrated fertilizer production facility in green hydrogen scenario by 2030

Fuel	Consumption speed	Unit
Electricity	5.13	TJ/ hour

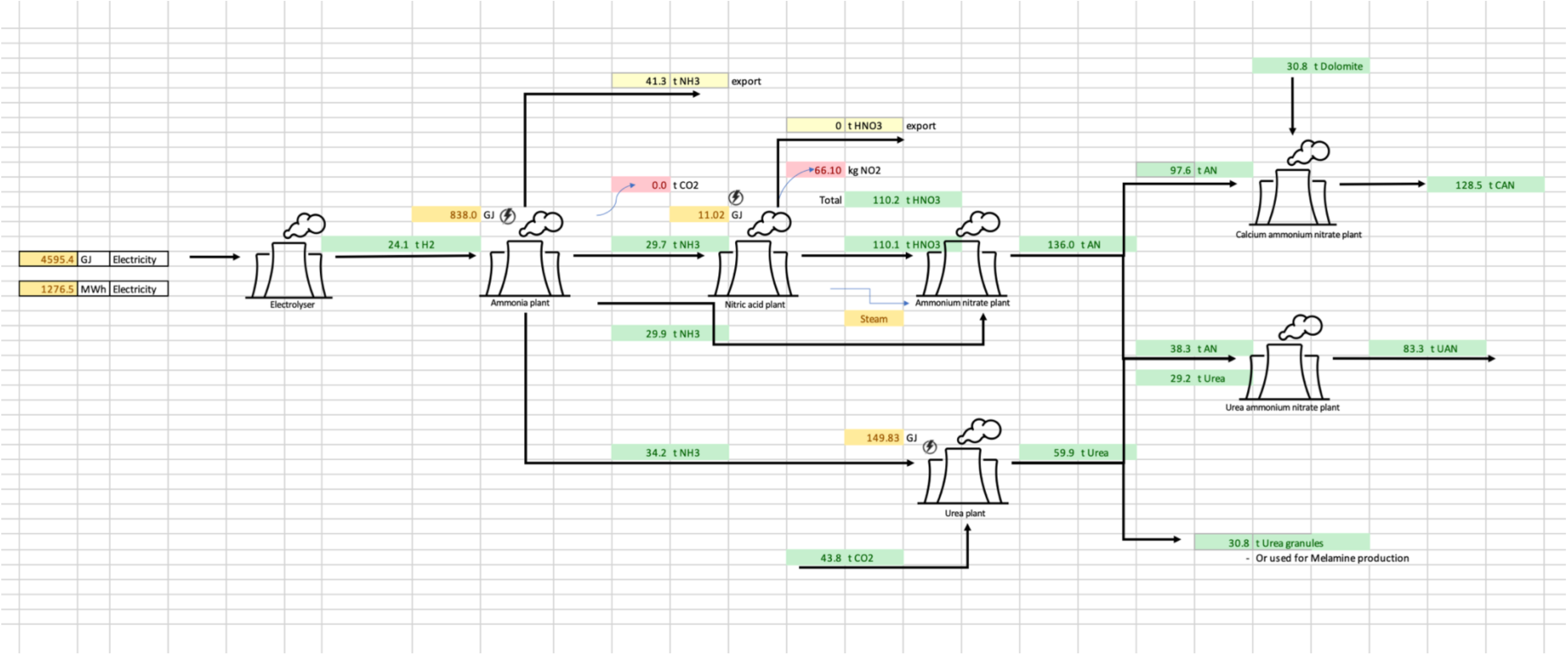


Figure 11. Hourly consumption and production profile of an integrated fertilizer plant in the Green Hydrogen scenario by 2030.

5.4 Conclusion

The estimated electricity demand of the ammonia, nitric acid and urea plant are determined for all three decarbonization pathways. The findings are presented in Table 24. Notably, moving from the BAU Scenario to the CCS Scenario requires an annual electricity demand increase of more than 300%. Moreover, moving from the BAU scenario to the Green Ammonia Scenario requires shift away from natural gas towards a 100-fold higher annual electricity demand.

Table 24. Annual electricity demand of the production plants in three scenarios.

Annual electricity demand	BAU Scenario [GWh]	CCS Scenario [GWh]	Green Ammonia Scenario [GWh]
Ammonia plant	60.1	60.1	1862
Nitric acid plant	24.5	24.5	24.5
Urea plant	39.9	39.9	333
CCS system	-	271.5	-
Electrolyzer	-	-	9188

From the annual electricity demand in combination with the estimated production activities of an existing fertilizer production facility, the hourly electric load is determined for a fictive fertilizer production facility by 2030. How the decarbonization pathways alter the hourly electricity requirements of a fertilizer production plant is shown Table 25. In Table 25 the electric capacity of the electrolyzer is presented separately to clearly show where the electricity is needed in the system. However, in previous notations, the energy requirements for methane-fed hydrogen production are considered part of ammonia synthesis. Therefore, the energy requirements to produce one tonne ammonia include the electricity requirements of the electrolyzer in future sections.

Table 25. Hourly electric capacity the production plants in three scenarios.

Hourly electricity loads	BAU Scenario [MW]	CCS Scenario [MW]	Green Ammonia Scenario [MW]
Ammonia plant	7.5	7.5	233
Nitric acid plant	3.1	3.1	3.1
Urea plant	5.0	5.0	42
CCS system	-	34	-
Electrolyzer	-	-	1149

6 Specific energy costs

6.1 Historic energy costs and ammonia prices

Following, the specific production costs of fertilizer products are determined to estimate the economic impact of a decarbonized fertilizer production route and to answer the third sub research question: “how do the decarbonization pathways alter the production costs of nitrogenous fertilizer products?”. Since fertilizer products are predominantly produced from hydrogen and nitrogen, the production costs are merely depended on the price of natural gas, electricity, and CO_2 permits. Inevitably, one would expect the price of ammonia to be correlated to its feedstock prices. Schnitkey (2016) examined the correlation between the US ammonia price and national natural gas price developments, as shown in in Figure 12.

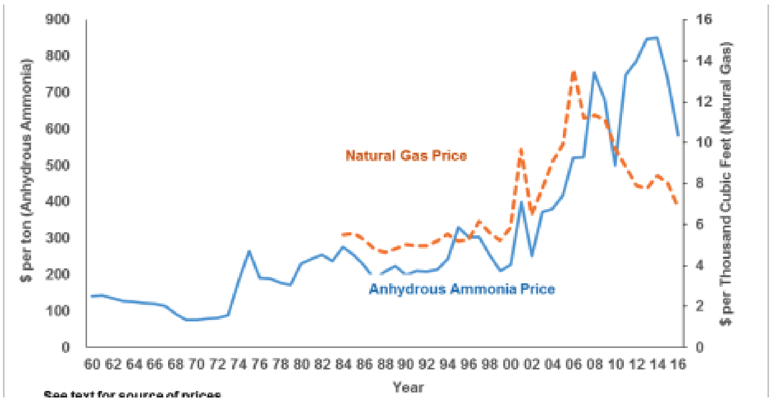


Figure 12. Historic price data of US anhydrous ammonia prices and national natural gas price developments (Schnitkey, 2016)

Their findings presented that between 1984 and 2006 the correlation coefficient of the relationship between natural gas and anhydrous ammonia prices happened to be 0.90 (Schnitkey, 2016). In other words, the closer this correlation coefficient comes to 1, the more the national ammonia prices follow the price rate of natural gas accordingly. Calculating the same correlation coefficient between 1984 and 2016 resulted in a value of 0.67 (Schnitkey, 2016). Ultimately, after 2006, more factors determining anhydrous ammonia prices came into place, e.g., the demand of agricultural food products. Following, averaged historic ammonia costs are estimated to examine the relationship between energy costs and ammonia prices. Figure 13 presents historical price data of averaged natural gas, and CO_2 permits of the EU-27 (Eurostat, 2022a, 2022b; Trading Economics, 2022) and estimated EU-27 whole-sale yearly electricity prices by averaging hourly electricity prices from The Netherlands, Spain, Greece, and Sweden between 2015 and 2022 (Entsoe, 2022).

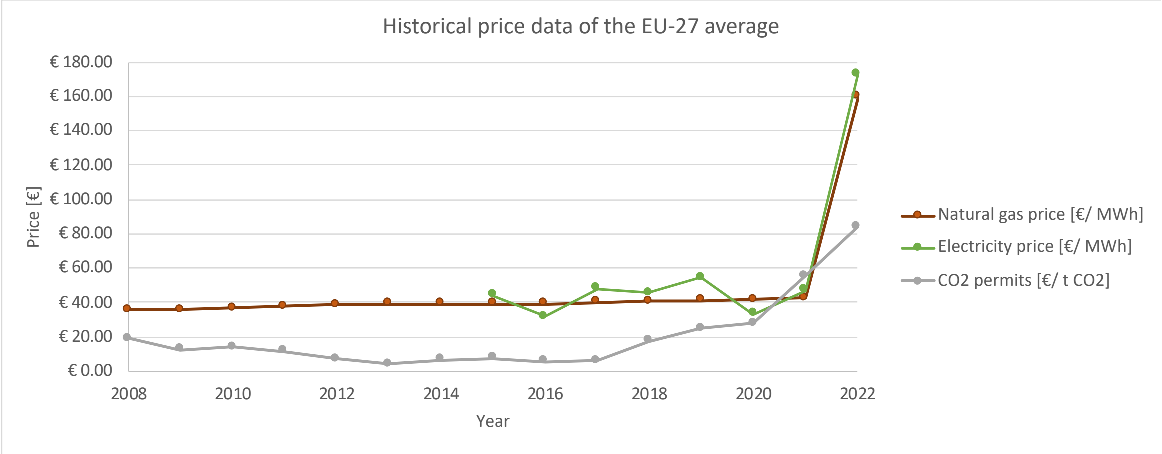


Figure 13. Historical price data of natural gas, electricity, and carbon permits of the EU-27 (Entsoe, 2022; Eurostat, 2022b; Trading Economics, 2022)

Concerning above presented price data of natural gas, electricity and carbon permits, the profitability of anhydrous ammonia is estimated over the last 12 years. Since public data lacks historic trends of European anhydrous ammonia prices, averaged prices of anhydrous ammonia are retrieved from Schnitkey et al. (2021), thus based on the anhydrous ammonia market of the United States. The profit margin of anhydrous ammonia is presented in Figure 14. Figure 14 shows that since 2021 natural gas prices and carbon permits have risen substantially compared to the past which continued up to a level where in some cases the production of ammonia is not beneficial anymore. Since the invasion of Ukraine in February 2022, European ammonia production costs exceeded European ammonia resell prices (Schnitkey et al., 2022). These kinds of trends forced Yara Sluiskil to shut down their ammonia production plants due to soaring natural gas prices (McDonald, 2022).

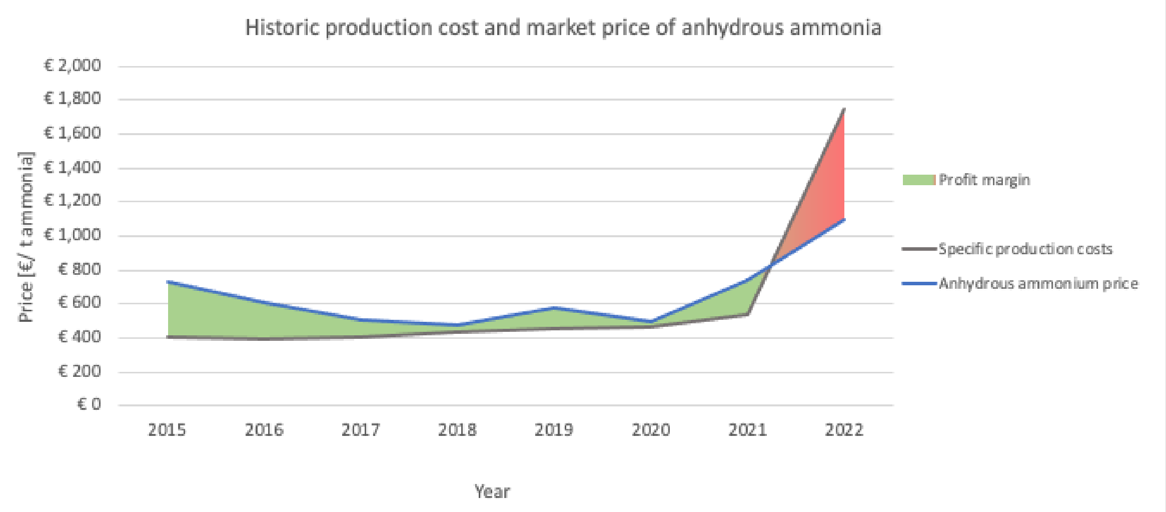


Figure 14. Historical production cost and market price of anhydrous ammonia (Schnitkey, 2016)

6.2 Future projections of energy costs

To estimate the energy cost for the production of ammonia, natural gas and electricity prices, and CO_2 permits are estimated for 2030. Projections on natural gas prices are not considered very precise due to a tremendous number of assumptions. The price of carbon permits by 2030 are based on the recommended carbon-pricing of the UN-Convened Net-Zero Asset Owner Alliance. Their discussion paper on governmental carbon pricing mentioned that OECD require a central estimate of €120 per tonne by 2030 to facilitate net-zero emissions by 2050 (UN-Convened Net-Zero Asset Owner Alliance, 2021). Therefore, carbon pricing at €120 per tonne could be considered a high-end CO_2 price. To determine the effect of rising CO_2 permit prices from almost €40 per tonne CO_2 in 2020 to €80 per tonne CO_2 in the beginning of 2022 (Trading Economics, 2022), three carbon pricing scenarios are examined. BAU 40, BAU 80 and BAU 120 refer to the BAU producing route with carbon pricing of €40, €80, and €120 per tonne CO_2 respectively. Over the last decade, carbon permits used to be lower than €20 per tonne CO_2 but showed rising price over the last few years. Therefore, BAU 40 represents the expected minimum carbon price following by the BAU 80 being the 2022 average and BAU 120 representing the high end 2030 carbon price estimated by the United Nations. In the CCS scenario, the price of carbon remained €120 per tonne CO_2 since the impact of carbon permits with a 96% CO_2 emission reduction compared to the BAU is considered negligible.

Electricity price data is retrieved from the METIS studies of the European Commission. METIS is mathematical simulation model which analyses the European energy system for electricity, heat, and gas to simulate the operation of energy systems on an hourly basis. Relative to the Reference Scenario 2020, the European Commission has produced three policy scenarios as a measurement tool to analyses the impact of various initiatives of the Green Deal Policy package. One of these three scenarios is the MIX scenario which relies on strong intensification of energy and transport policies as well as carbon price signal extension to road transport and buildings (European Commission, n.d.). Projections of the MIX scenario and the associated electricity prices in 2030 are simulated with the METIS model. Although the details about the MIX-2030 scenario are published publicly, the output of the METIS model is still confidentially, therefore, hourly electricity prices will not be published in this research paper.

Considering the energy consumption profile of a fertilizer production facility in 2030, the specific costs of ammonia production are estimated for varying prices of natural gas and CO_2 permits. Since the Green Ammonia scenario merely consumes electricity and does not lead to direct CO_2 emissions, the production costs of 1 tonne ammonia is constant for varying prices of natural gas and CO_2 permits. Due to hourly fluctuating electricity prices in the simulation of the MIX-2030 scenario, the electricity costs to produce 1 tonne ammonia in the Green Ammonia Scenario, are estimated by taking the yearly average. The production costs of ammonia in the BAU, CCS and Green Ammonia scenario are presented in Figure 15.

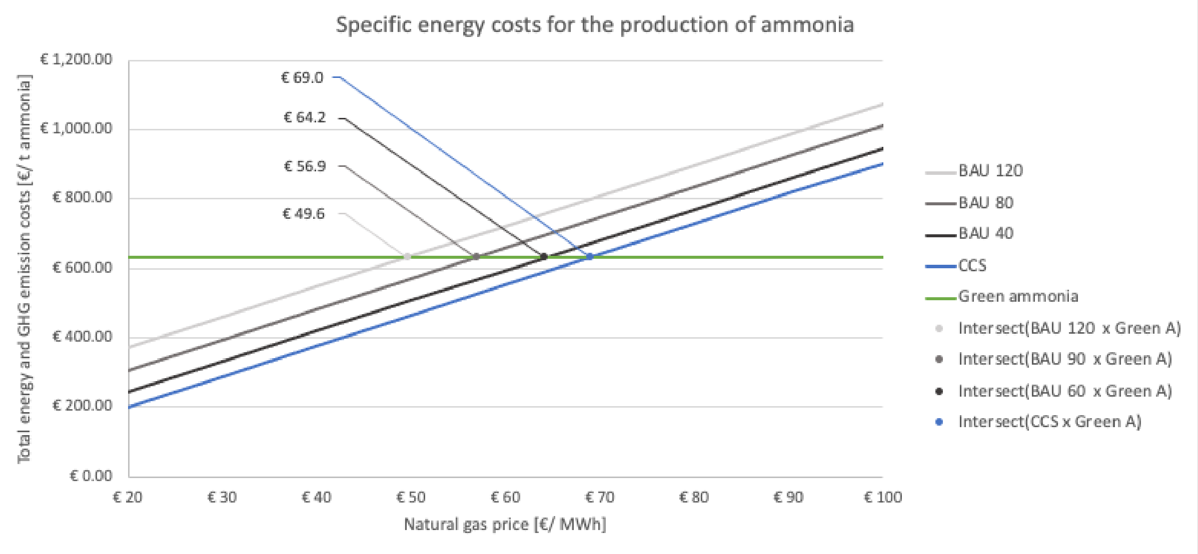


Figure 15. Specific energy costs for the production of ammonia with varying prices of natural gas.

Considering a carbon pricing scheme of €40, €80, and €120 per tonne and the electricity price data of the MIX-2030 scenario in the Netherlands, in future scenarios, green ammonia will only be profitable when natural gas prices are higher than the intersection of scenarios as presented in Figure 15. In other words, a fully electrified ammonia production process can be considered less cost intensive compared to the BAU 40, BAU 80 and BAU 120 and CCS production route when natural gas prices are higher than €64.2, €56.9, €49.6, and €69 per MWh respectively. However, due to current geopolitical conflicts, natural gas price fluctuations make it rather complex to make future projections with regards to averaged European energy prices. Over the last year, natural gas prices have risen by 500% becoming the driving force of global inflation and the new 'Cold War' (Freitas Jr et al., 2022). Figure 16 presents Dutch natural gas prices in euro per MWh over the last year. Since September 2021, European natural gas prices have exceeded €50 per MWh. From this point onwards, natural gas prices have fluctuated significantly with already 400% price increase in November 2021 compared to the start of year. In addition, the invasion of Ukraine by Russia is clearly visible in Figure 16, where a spike of €216 per MWh occurred between February and March 2022 (Sönnichsen, 2022b). Ultimately, these daily fluctuations and an instable market have led to an unpredictable future for natural gas prices.

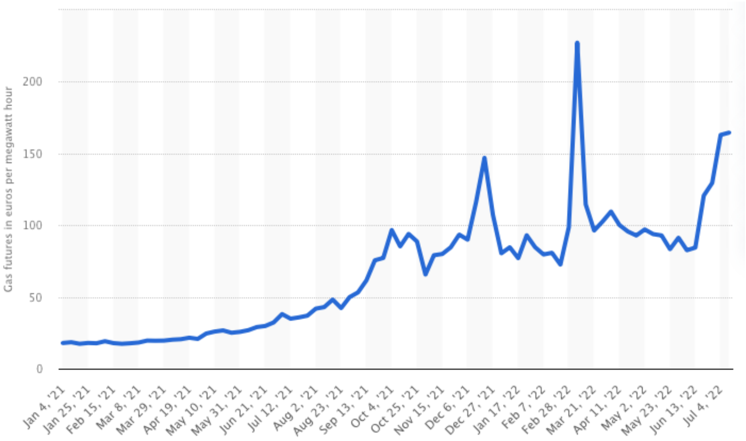


Figure 16. Dutch TTF gas futures at the beginning of each week from January 4, 2021, to July 11, 2022 (Sönnichsen, 2022b)

Concerning this instable and unpredictable natural gas market, future projects should be made with multiple scenarios. The total energy costs and CO_2 pricing are presented in Table 26. Table 26 shows that in a scenario where one MWh natural gas cost €40 like in a period before September 2021, the BAU and CCS scenario are significantly lower in production costs compared to the Green Ammonia scenario. However, these costs do not include the investment costs needed to build an electrified production plant. Nevertheless, in scenarios where natural gas prices are close to the past 6 months with an average of approximately €90 per MWh or even at current level of €160 per MWh, a full electrified fertilizer production facility is substantially lower in operational costs annually.

Table 26. Total annual production cost based on natural gas and electricity prices, and carbon pricing.

Annual energy costs and CO_2 pricing		Total cost (€40/ MWh natural gas) [M€]	Total cost (€90/ MWh natural gas) [M€]	Total cost (€160/ MWh natural gas) [M€]
BAU Scenario	€40/ t CO_2	€ 457	€ 931	€ 1,595
	€80/ t CO_2	€ 526	€ 1,000	€ 1,665
	€120/ t CO_2	€ 595	€ 1,069	€ 1,734
CCS Scenario	€120/ t CO_2	€ 412	€ 886	€ 1,551
Green ammonia Scenario		€ 704	€ 704	€ 704

Furthermore, the production costs per tonne of product are displayed for three different natural gas prices versus three different carbon pricing scenarios in the BAU scenario compared to the Green Ammonia scenario. At first, concerning past trends in Figure 13, the past average is assumed to be €40 per MWh natural gas. Secondly, based on last the trend of last 12 months, the average natural gas prices of the present are assumed to be €90 per MWh. Lastly, concerning a remaining tension of geopolitical games related to the current maintenance period of Nord Stream 1, the third natural gas price scenario sets the price of natural gas at the July 2022 level of €160. In combination with the electricity data of MIX-2030 scenario and a carbon pricing of €40, €80, and €120 per tonne CO_2, the production cost of 1 tonne of product is presented in Figure 17. The estimated price of calcium ammonium nitrate includes the assumption that by 2030 the price of Dolomite will remain at the 2021 level, i.e., €39 per tonne (IndexBox Inc, 2022). Figure 17 visualizes how varying carbon pricing and natural gas prices affect the production costs of 1 tonne of product. These findings show that an increase of carbon permits from €40 to €80 per tonne CO_2 with a constant natural gas price, results in a product cost increase of approximately 15%. Whereas a natural gas price increase from €40 to €90 per MWh with a constant carbon permit price led to a production cost increase of more than 100%. Ultimately, the dominant variable determining whether the Green Ammonia production route results in a production cost reduction compared to the BAU production route happens to be the natural gas price.

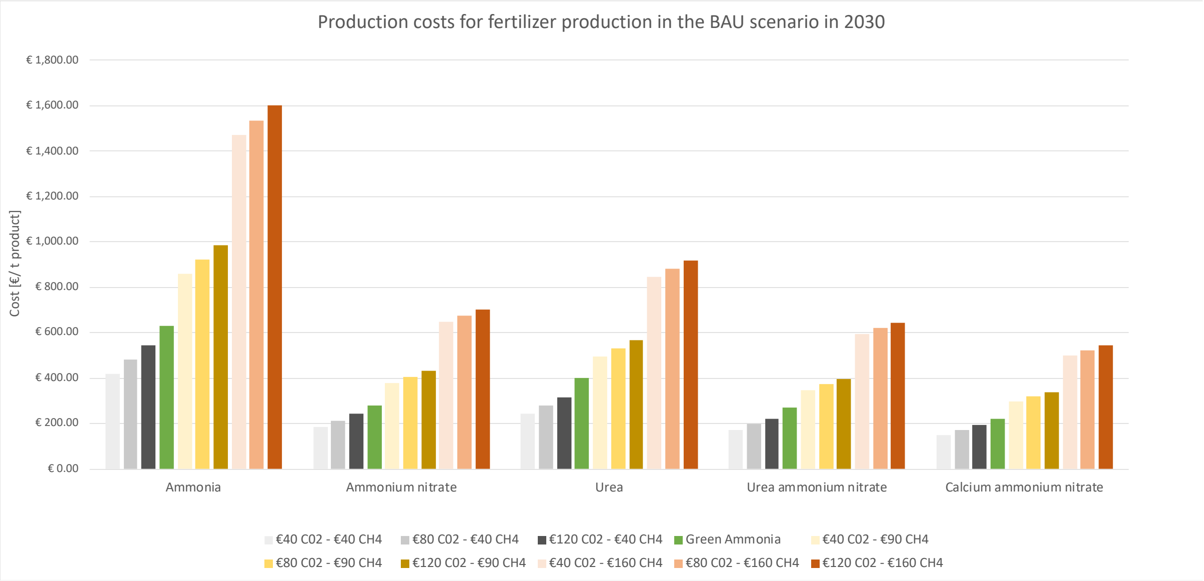


Figure 17. Production cost for fertilizer production in 2030 of the BAU scenario with a varying natural price of €40, €90, and €160 per MWh and varying carbon permit prices of €40, €80, and €120 per t CO_2 compared to the Green Ammonia Scenario. The electricity consumption in the electrolyzer is included in the total energy cost per tonne ammonia in the Green ammonia scenario.

Based on above presented findings, by 2030 the carbon pricing is assumed to be €120 per tonne CO_2 emitted since the United Nations presented this as the necessary to achieve the 2030 goals. Following, the production costs of fertilizer production is presented in Figure 18 for three production routes concerning a varying natural gas price. Figure 18 shows that a rising price of natural gas significantly increase the production costs of (intermediate) fertilizer products. Moreover, since ammonia is considered the main input of all the other intermediate and final products, the specific energy cost of this (intermediate) fertilizer product is almost negligible compared to the cost of the required amount of ammonia. In the Green ammonia scenario, the electricity consumption in the electrolyzer is considered part of the ammonia production process, thus included in the graph. Although predicting future natural gas prices is currently considered rather complex, in the next chapter, the natural gas price is assumed to be €90 per MWh by 2030.

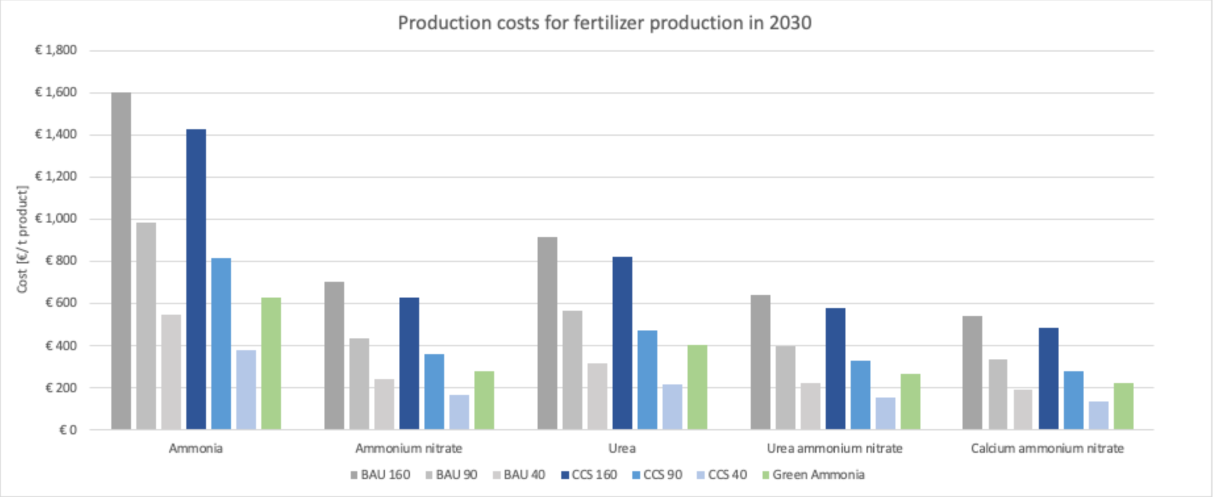


Figure 18. Production cost for fertilizer production in 2030. BAU 160 refers to the BAU scenario with a natural price of €160 per MWh. The electricity consumption in the electrolyzer is included in the total energy cost per tonne ammonia in the Green Ammonia scenario.

7 Utilization of demand side management tools

In this section, the technical and economical DR potential of low-carbon fertilizer plants are determined to answer the fourth and fifth sub-research questions. This research examines the DR potential of the business-as-usual (BAU) scenario and two decarbonization pathways. The assumption is made that the decarbonizations strategies have been implemented before 2030. Therefore, when estimating the technical and economic potential of DR application in the different scenarios, investment costs of implementing clean energy technologies in existing fertilizer plants or investment costs of building a whole new low-carbon fertilizer production plant will not be taken into consideration.

Using the energy demand profiles of the BAU and the decarbonization scenarios obtained in previous section, the theoretical DR potential will be determined by using the following 4 step approach of the decomposition method of (Dranka & Ferreira, 2019).

1. Identification of the processes suitable for DR for each sector (i.e., ammonia, nitric acid, ammonium nitrate and urea production).
   In chapter 5 suitable processes for DR are determined for all three scenarios.
2. Quantification of electricity loads: Calculation of the annual electricity demand and the maximum installed capacity.
   Table 24 and Table 25 from section 5.4 present the annual electricity demand and the maximum installed capacity. Since all processes are continuous process that always run at full speed, under normal conditions, the hourly electricity load is considered its maximum capacity
3. Quantification of daily load profile for each process.
   As mentioned earlier, all processes are continuous processes that always run at full speed. Therefore, the daily load profile contains 24 hours of continuous production.
4. Quantification of hourly electricity demand

Following, the technical DR potential will be estimated with the following steps

5. Technical constraints
6. Optimization Modelling Approach

<u>Technical constraints:</u>

- Storage capacity: the production of fertilizers is dependent on the production of multiple intermediate products (e.g., ammonia and nitric acid) therefore the production speed of ammonium nitrate and urea relies on the storage capacity of these intermediate products. The production of intermediate products must not exceed its maximum storage capacity and the production speed of final products must not exceed the production speed of intermediates and available stored intermediates combined
- Installed capacity: the production speed could be ramped up or down to minimize the cost of electricity depending on the capacity factor of the installed capacity of the fertilizer plant
- Ramp up/ down rate: the load shift potential of a production step depends on whether the process is a continuous process and if it is bound to minimum or maximum production speed. Inevitable, flexible production is determined by the capabilities of a production process to alter its standard production properties.
- It is important to consider the that during sow of seeds the demand for fertilizers are high. Therefore, seasonal variations of fertilizer demand are considered for the technical restrictions with regards to the planning of the annual maintenance period.

Following, the economic DR potential will be estimated with the following steps

7. Economic drivers
8. Optimization Modelling Approach

Economic drivers:

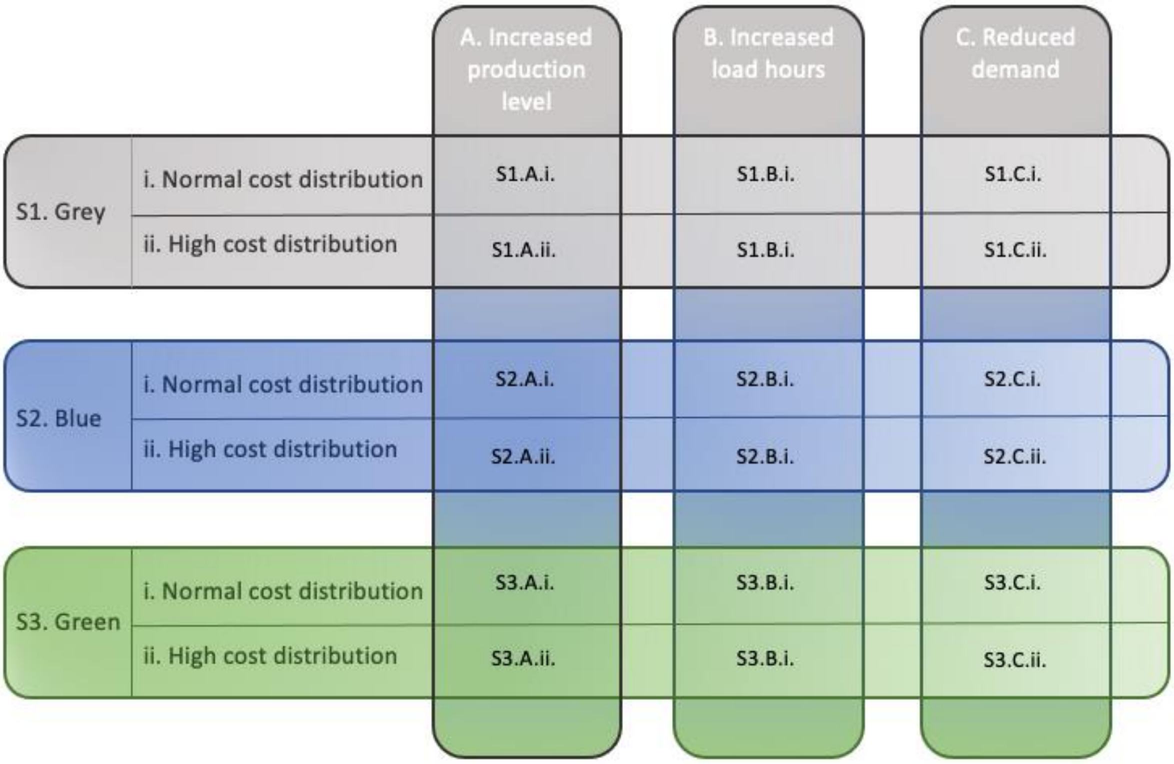
- Historical electricity price data does provide insides in daily fluctuation of electricity prices. However, this data does not take the influence of a high renewable share in the fuel mix and the associated intermittency on hourly electricity prices into account. Therefore, electricity price data is retrieved from the MIX-2030 scenario METIS studies of the European Commission.

Optimization modelling

A linear program will be used to optimize the objective function. This research contains an objective function the aims at minimizing the linear problem to find the minimum electricity costs of a fictive fertilizer plant.

All linear programming steps are developed in Spyder. Spyder is an open-source scientific environment that is written in Python which can be accessed via the Anaconda-Navigator. The optimization modelling is performed with the PuLP module which allows you to create a model object by adding variables and constraints and solve the linear problem with pulp.lpSum() in the PuLP package

The linear program is optimized in eighteen scenarios as presented in Figure 19. The eighteen different scenarios are determined by a matrix of the BAU (S1), CCS (S2) and Green Ammonia (S3) scenarios as described in chapter 5, the varying production profile scenarios (A, B, and C) which are described in chapter 7.1, and the electricity cost distribution scenarios (i and ii) which are described in chapter 7.2.



		A. Increased production level	B. Increased load hours	C. Reduced demand
S1. Grey	i. Normal cost distribution	S1.A.i.	S1.B.i.	S1.C.i.
	ii. High cost distribution	S1.A.ii.	S1.B.i.	S1.C.ii.
S2. Blue	i. Normal cost distribution	S2.A.i.	S2.B.i.	S2.C.i.
	ii. High cost distribution	S2.A.ii.	S2.B.i.	S2.C.ii.
S3. Green	i. Normal cost distribution	S3.A.i.	S3.B.i.	S3.C.i.
	ii. High cost distribution	S3.A.ii.	S3.B.i.	S3.C.ii.

Figure 19. Visualization of the sixteen scenarios in which the linear program is optimized to find the most cost-efficient fertilizer production route.

7.1 Technical demand response potential

Concerning the target in the Paris Agreement to become carbon neutral by 2050, renewable energy sources will be predominantly exploited in the power sector to reach the almost 100% renewable fuel mix. Therefore, the distribution of energy on the grid will face some endeavors with regards to regional imbalances due to intermittent regional supply. Demand-side management tools have the potential to match the demand and supply. According to Dranka & Ferreira (2019), the technical demand response potential is defined as the overall consumers' potential considering technical restrictions such as shifting time, duration, and boundaries. In this section, the constraints of technical demand response potential will be determined to answer the third research question: *"What is the technical demand side response potential of a low-carbon nitrogenous fertilizer production plant?"*

7.1.1 Storage capacities

At first, to participate in demand response, it is favored for fertilizer production facility to have a storage possibility for all intermediate products (Kelley et al., 2022), i.e., ammonia, nitric acid, urea, and ammonium nitrate. The storage quantity of a product in the corresponding storage tank is often expressed as S, where S_t represents the stored quantity at time t and S_{max} represents the maximum storage capacity. At all times, the storage level of a product at time t must never exceed the minimum and maximum installed capacity of the storage tank, as shown in Equation 1:

$$0 \leq S_t \leq S_{max}, \forall t \qquad \text{[Eq. 1]}$$

Storage of liquid ammonia is not an energy intensive process and requires only 0.6% of its energy (Dias et al., 2020). Ammonia is often stored at ambient temperature and 8 bar pressure or at atmospheric pressure at -33 ˚C (Dias et al., 2020). The ammonia storage tank is assumed to be 33 kt which is similar to the storage capacity of 30 kt of the storage tanks acquired by OCI in Rotterdam. In addition, at the OCI Beaumont facility, 331 kt ammonia (final product) is produced annually which equals the annual production of 331 kt ammonia (final product) at the facility in Geleen. At OCI Beaumont, the current installed storage capacity of two tanks combined is 33 kt (OCI N.V., 2016).

Another fertilizer production facility of OCI located in Iowa, called Iowa Fertilizer Company, produces urea and urea-ammonium nitrate with an annual production of 420 and 1505 kt final product respectively. At this facility, urea and urea-ammonium nitrate are stored in storage tanks with a storage capacity of is 44 kt and 132 kt respectively (OCI N.V., 2016). For these two products, the installed storage capacity is approximately 10% of the annual production of urea and urea-ammonium nitrate. Concerning intermediate products, this 10% only relates to the annual production of a product as a final product without taken the consumption of the same product for a following production process into consideration. These two examples in combination with the example at OCI Beaumont lead to the assumption that the fictive European fertilizer plant is likely to have an installed storage capacity equal to 10% of the annual production of a final product. Since nitric acid and ammonium nitrate are not considered final products, there is assumed that by 2030 nitric acid and ammonium nitrate can be stored in storage tanks. The installed storage capacity is calculated with the same ratio of storage capacity of ammonia versus total production of ammonia, being 3%.

Only two technologies are currently considered suitable for large scale hydrogen storage: liquified hydrogen storage and geological underground compressed hydrogen storage. Liquified hydrogen storage has the disadvantage that investment cost per tonne hydrogen stored are estimated to be at least one order of magnitude more capital intensive compared to geological underground storage (Davies et al., 2020). Moreover, to keep hydrogen in the liquid state, hydrogen should be cooled under -253 ˚C which is considered quite an energy intensive process requirement (Davies et al., 2020). Underground compressed hydrogen storage is currently utilized in the Clemens and Moss Bluff caverns in Texas with an estimated storage capacity of 2500 tonnes and 3700 tonnes of hydrogen respectively (Davies et al., 2020). The disadvantage of hydrogen stored underground in salt caverns is that it requires the presence of these caverns. For this research there is assumed that by 2030 a fertilizer production facility will have an installed hydrogen storage capacity in the same ratio as its ammonia storage tank, i.e., 5.8 tonnes of hydrogen stored underground. The installed storage capacities of the fictive fertilizer production facility are presented in Table 27.

Table 27. Installed storage capacity of intermediate and final products

Product	Annual production (kton)	Final product (kton)	Storage capacity (kton)
Ammonia	1081	331	33
Nitric acid	881	-	27
Ammonium nitrate	1087	-	33
Urea	479	246	25
UAN	667	667	67
CAN	1028	1028	103
Hydrogen	192	-	5.8

7.1.2 Installed capacity

Secondly, the technical demand response potential depends on the maximum installed capacity of the production plants. The maximum installed capacity of a production plant determines the maximum production level of the plants, hence, its possibility to produce at either a lower or a higher production level compared to the conventional production profile. A continuous running chemical production plant has a minimum production speed due to its internal heat at which catalytic processes take place. Therefore, a chemical production plant may never be ramped down below its own minimum production speed. All production steps of the integrated fertilizer production facility are considered continuous production processes. According to personal communication with OCI, the steam methane reforming reactors may never produce at a lower rate than 80% of their standard production speed (OCI N.V., 2022). Based on this data, the assumption is made that to produce ammonia, nitric acid, and urea, the minimum production level is set at 80% of their standard production level. The maximum production level of the ammonia, nitric acid plant is determined in the following three scenarios.

A. Increased production scenario

In this research, the average production speed is estimated based on the report of (Batool & Wetzels, 2019) who estimated the annual production of OCI with 8000 load hours. To produce flexibly, for instance at a lower rate during high electricity prices, the production facility must also be able to produce at higher rate compared to the average. The book volume Chemical Engineering Design of Coulson & Richardson's Chemical Engineering present all design factors that ensure the safety of a plant. When designing a production plant, design specifications must be met to provide a margin of safety ensuring the performance of equipment. The maximum flows for equipment instrumentation, and piping design is typically calculated with an increased factor of 10% (Sinnot, 2005, p. 13). In other words, the calculated production level of a plant running at full speed during all its load hours could in theory be increased by 10% while still ensuring satisfactory performance of equipment. Therefore, in this scenario there is assumed that by 2030, the max production level of the ammonia, nitric acid and urea plant is 110% compared to the average 2020 production level.

B. Increased load hours scenario

Instead of 8000 operating hours a year with an increased production capacity, the number of load hours the production plants run could be increased to implement flexible production possibilities. In reality, maintenance is planned only ones every 3 years, instead of every year (OCI N.V., 2022). This would lead to 8760 load hours annually. In combination with a constant demand for fertilizer products, producing for 8760 hours between 80% and 100% of the average production speed could also have a peak-load shifting effect.

C. Reduced demand scenario

The last scenario is meant to show whether a changing demand for fertilizer products could provide a load shift potential which potentially outbalancing the profit loss caused by less products sold. Since the other two scenarios either have the assumption that the production speed might increase by 10% or an increase of 760 load hours annually, which in fact means a 9.5% increase of operation, this scenario assumes that the demand for fertilizer products is reduced by 10% in 2030 due to movements towards more sustainable farming practices. Therefore, the production plants can run between 80% and 100% of the average production speed for 8000 load hours with an annual production of 90% compared to standard conditions.

The minimum, average and theoretical maximum production levels in scenarios 1, 2 and 3 are presented in Table 28, Table 29, and Table 30 respectively.

Table 28. Range in production level of the production plants in the BAU-scenario.

Production process	Min production level BAU Scenario [MW]		Average production level BAU scenario [MW		Max production level BAU Scenario [MW}	
	MW	Percentage	MW	Percentage	MW	Percentage
Ammonia	6.0	80%	7.5	100%	8.3	110%
Nitric acid	2.4	80%	3.1	100%	3.4	110%
Urea	4.0	80%	5.0	100%	5.5	110%

Table 29. Range in production level of the production plants in the CCS-scenario.

Production process	Min production level CCS scenario [MW]		Average production level CCS scenario [MW		Max production level CCS scenario [MW}	
	MW	Percentage	MW	Percentage	MW	Percentage
Ammonia	6.0	80%	7.5	100%	8.3	110%
Nitric acid	2.4	80%	3.1	100%	3.4	110%
Urea	4.0	80%	5.0	100%	5.5	110%
CCS	0	0%	37.3	100%	41.1	110%

Table 30. Range in production level of the production plants in the Green Ammonia scenario.

Production process	Min production level Green scenario [MW]		Average production level Green scenario [MW		Max production level Green scenario [MW}	
	MW	Percentage	MW	Percentage	MW	Percentage
Ammonia	186	80%	233	100%	256	110%
Nitric acid	2.4	80%	3.1	100%	3.4	110%
Urea	33.3	80%	41.6	100%	45.8	110%
Electrolyzer	0	0%	1149	100%	1264	110%

7.1.3 Ramp up/ down rates

Besides storage possibilities, the maximum installed capacity, and the minimum and maximum production speed, the technical demand response potential is bounded by the load shift potential of the production processes. The load shift potential can be determined by the shifting time of a continuous or batch process.

Increasing or decreasing the production speed at t = 1 compared to t = 0, is limited by its ramp up/ ramp down rate. According to a short interview with Asset Performance Networks (2022), production facilities with an average use of catalytic reactions could ramp up or down their production speed with 5% compared to the standard production speed in approximately 4 hours. Therefore, the assumption is made that the ammonia, nitric acid, and urea plant are limited by a ramp up/ down rate of 1.25% per hour (Asset Performance Networks, 2022). The Carbon capture and storage system and the electrolyzer are assumed not to be bounded by a ramp up/ down rate (Bruns et al., 2022; Domenichini et al., 2013). Including a minimum and maximum production rate compared to their stand production rate could potentially lead to a load shift potential, which is visualized in Figure 20. The example of the ammonia plant in Figure 20 shows that the areas below both lines are equal, hence, the green area expresses the load shift potential of a flexible production facility.

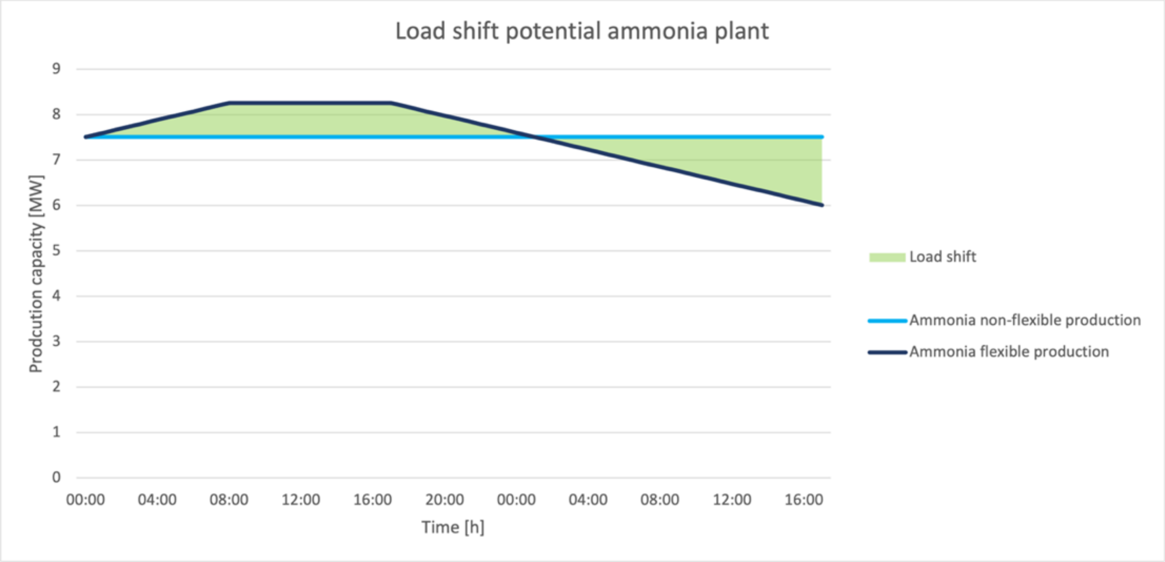


Figure 20. Load shift potential based on flexible production rates of the ammonia plant with an increased maximum production level.

7.2 Economic demand response potential

In this section, the constraints of the economic demand response potential are determined to answer the fourth sub-research questions: *"What is the economical demand side response potential of a low-carbon nitrogenous fertilizer production plant?".* The economic demand response potential is defined as the technical demand response potential plus the supposedly cost-effective overall consumers' potential (Dranka & Ferreira, 2019). In other words, within all scenarios, the overall consumption of energy will remain constant, while the hourly varying electricity consumption determines load shifting drivers and cost savings.

7.2.1 Electricity costs

For the simulations, electricity price data for 2030 is retrieved from the METIS studies of the European Commission. During the simulation the price of electricity sometimes becomes negative. Therefore, a constraint is included which does not allow the price of electricity to be lower than zero. Otherwise, energy providers must pay consumers for their energy consumption. Moreover, at nine timesteps in the simulation, the electricity price appeared to rise far above the average, i.e., €15,000 per MWh. However, governmental regulation and interventions will prevent this from happening. Therefore, another constraint is included stating that electricity prices must never exceed €500 per MWh. The demand response potential off all scenarios is modelled for two electricity price scenarios in 2030. One with a 'normal' electricity cost distribution and one with a relatively 'high' electricity cost distribution. The difference between these two electricity price simulations lies on the differences in climatic conditions in the year of simulation.

Since the fictive fertilizer production facility runs for 8000 hours annually, the electricity price data must be adjusted for the "increased production yield" and the "reduced demand" scenarios. Turnarounds in the Netherlands are often planned during spring or fall. Nitrogenous fertilizer products are predominantly applied on agricultural land during the beginning of March and the end of August (Ma et al., 2016). Since excessive rates of nitrogen fertilization could reduce crop yields, matching the timing and rates of fertilization is considered of great importance for yield maximization (Ma et al., 2016). Therefore, the assumption is made that a turnaround of the fertilizer production facility is planned in October. As a result, the time steps between September 30th 11 PM CEST, 2030 and November 1st 3 PM CEST, 2030 are left out in optimization scenarios with 8000 load hours annually. The average electricity price ± standard deviation of both the normal and high electricity price distribution data are presented in Figure 21. Figure 21 shows that the average of the normal and high electricity cost distribution differs by less than 10%. Moreover, the impact of a maintenance period in October only significantly affects the average electricity price in the normal electricity cost distribution implying that the month October is quite an average month with regards to electricity prices in the high electricity cost distribution.

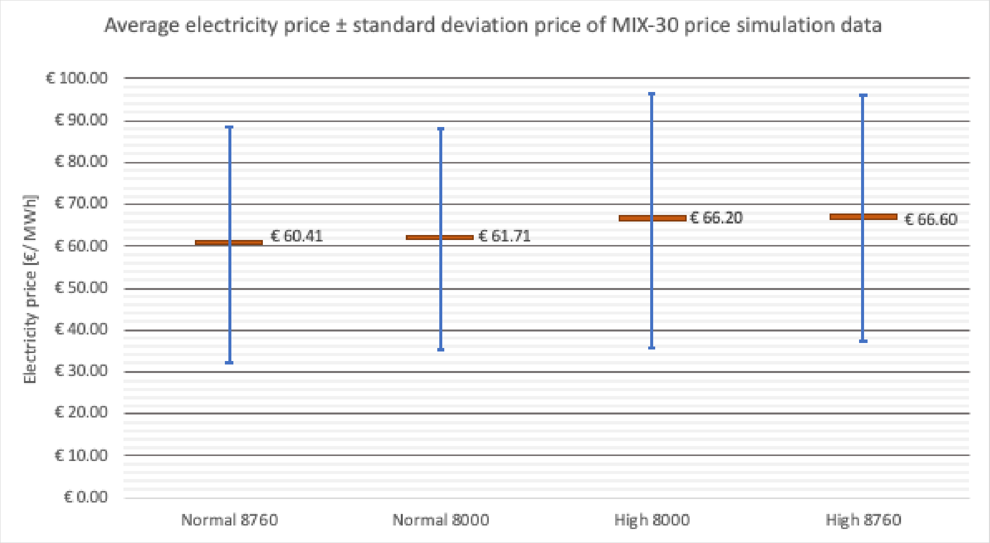


Figure 21. Average electricity price standard deviation of the normal and high electricity cost distribution data of the MIX-30 simulation.

7.3 Creating a model

Following, the technical and economic demand response potential are merged in a linear programming problem. Linear programming provides a method to achieve the most desirable outcome of a mathematical model. Within this model, linear relationships are represented by a set of decisions in a constrained environment. Linear programming is often used as a linear optimization tool to find the most cost-effective (cost minimization) or most profitable (profit maximization) outcome. This linear problem is the linear objective function where the system is defined by linear constraints using a varying set of decision variables. This linear programming model has the aim (LpProblem) to minimize the objective function (LpMinimize). The objective function is presented in Equation 2:

$$minimize \sum_t^T \sum_p^P E_t * C_{p,t} \qquad [Eq. 2]$$

The linear programming problem is created with the python library PuLP. Based on a set of parameters, the boundaries and input values of the system are defined. The input parameters are presented in the Table 31.

Table 31. Input parameter of the linear programming model.

Input parameter	Definition	Unit
C^{min}_p	Maximum hourly energy consumption of process p	MW
C^{min}_p	Minimum hourly energy consumption of process p	MW
eta_p	Conversion rate from Flow-in to Flow-out of process p	-
R^{up}_p	Hourly ramp up rate of process p	MW
R^{down}_p	Hourly ramp down rate of process p	MW
sec_p	Specific energy consumption of process p	MWh/ ton
S^{max}_p	Maximum storage capacity of process p	ton
S^{min}_p	Minimum storage capacity of process p	ton
$ProdminT_p$	Annual production of a product in process p	ton
E_t	Electricity price at time t	€ / MWh

Subsequently, the linear constraints within the system are defined by the following set of decision variables, Table 32.

Table 32. Decision variables of the linear programming model.

Decision variables	Definition
$C_{p,t}$	Electricity consumption of process p at time t
$S_{p,t}$	Storage of output product of process p at time t
$Fin_{p,t}$	Mass flow in process p at time t
$Fout_{p,t}$	Mass flow out process p at time t

Depending on the scenario of the future fertilizer plant, the process is divided into five processes. Python starts counting at 0, therefore, the first process is process 0 and the timesteps start at t = 0. Process 0 is ammonia production, process 1 is nitric acid production, process 2 is urea production, and process 3 is export of ammonia. In BAU scenario, process 4 are the CO_2 emissions of the ammonia plant, in the CCS scenario process 4 is the carbon capture and storage system with $Fout_{4,t}$ being the emission of the uncaptured CO_2, and in the Green ammonia scenario there are no direct CO_2 emissions, thus process 4 is production of hydrogen in the electrolyzer. Figure 22 presents a visualization of the system of the linear programming model.

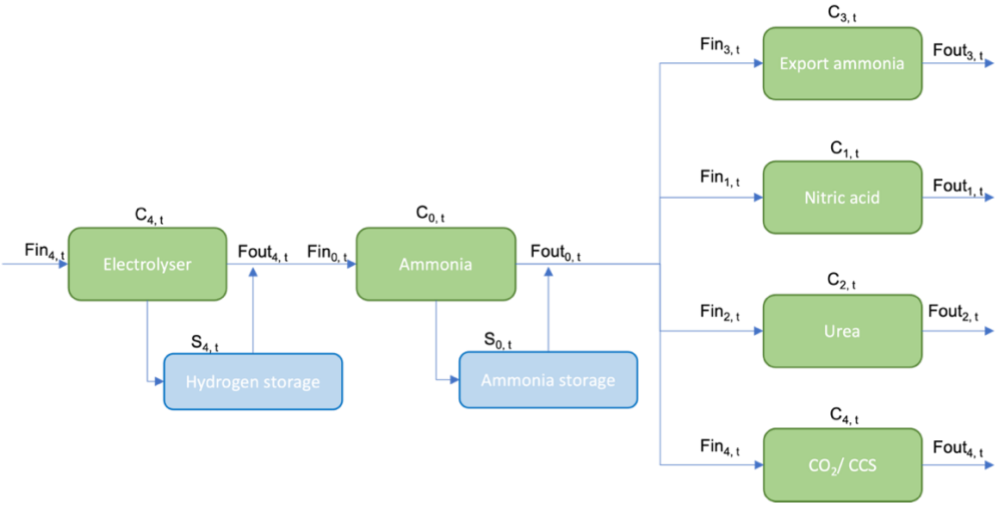


Figure 22. Visualization of the relationship between the decision variables and the processes.

Ammonia is used for nitric acid and ammonium nitrate production. Since the ammonium nitrate production does not require any additional electricity, the ammonia consumed for ammonium nitrate production is added to the process of nitric acid production. This is now considered one plant with an ammonia input of 0.27-ton per ton nitric acid and. With 1-ton nitric acid you can make 1.23-ton ammonium nitrate which requires an additional 0.272-ton ammonia. The model assumes that 1-ton nitric acid requires 0.54-ton ammonia and the same amount of electricity.

The following equations represent all the constraints used to solve the linear problem.

Constraint on energy consumption limits:

$$c_{p,t} = Fout_{p,t} * sec_p \quad \forall\, p, t \tag{Eq. 3}$$

$$C_p^{min} \leq c_{p,t} \leq C_p^{max} \quad \forall\, p, t \tag{Eq. 4}$$

$$c_{p,t} + R_p^{down} \leq c_{p,t+1} \leq c_{p,t} + R_p^{up} \quad \forall\, p, t \tag{Eq. 5}$$

Constraint on annual production requirements:

$$\textstyle\sum_t^T Fout_{p,t} = ProdminT_p \qquad \forall\, p \tag{Eq. 6}$$

Constraint on installed storage capacity:

$$s_p^{min} \leq s_{p,t} \leq s_p^{max} \qquad \forall\, p, t \tag{Eq. 7}$$

Constraints on mass flows in BAU and CCS scenario:

$$Fout_{p,t} = Fin_{p,t} * eta_p \qquad \forall\, p, t \tag{Eq. 8}$$

$$Fout_{0,t} + s_{0,t} - s_{0,t-1} = Fin_{1,t} + Fin_{2,t} + Fin_{3,t} \qquad \forall\, t \tag{Eq. 9}$$

$$Fout_{0,t} = Fin_{4,t} * 1.7 \qquad \forall\, t \tag{Eq. 10}$$

Constraints on mass flows in Green Ammonia scenario:

$$Fout_{p,t} = Fin_{p,t} * eta_p \qquad \forall\, p, t \tag{Eq. 11}$$

$$Fout_{0,t} + s_{0,t} - s_{0,t-1} = Fin_{1,t} + Fin_{2,t} + Fin_{3,t} \qquad \forall\, t \tag{Eq. 12}$$

$$Fout_{4,t} + s_{4,t} - s_{4,t-1} = Fin_{1,t} + Fin_{1,t} \; \forall\, t \tag{Eq. 13}$$

7.4 BAU Scenario output

In the BAU Scenario, the linear programming model is run for six different scenarios to quantify the load shift potential during normal and high electricity cost simulation and the impact of three flexible production strategies, as presented in Figure 19. The output of the linear programming model for all scenarios from S1.A.i – S1.C.ii are presented in section 12.1. In the 110% maximum production level scenario, the production of ammonia, nitric acid and urea tends to run predominantly at either maximum speed or at minimum speed, whereas, in both the increased load hours and reduced demand scenario the production speed also shows minor fluctuations at different levels to achieve minimum costs optimization. Furthermore, during the start of the year the price of electricity happens to be relatively high compared to the yearly average, hence, the plants tend to minimize their production speed in this period.

Table 33. Electricity cost for the production of ammonia, nitric acid and urea in the BAU production scenario.

Annual electricity cost [Million Euro}		Increased production level(110%)			Increased load hours (8760)			Reduced demand (90%)		
		Non-flexible [M€]	Flexible [M€]	Δcost	Non-flexible [M€]	Flexible [M€]	Δcost	Non-flexible [M€]	Flexible [M€]	Δcost
BAU	Normal price	7.68	7.46	-2.96%	7.52	7.30	-2.88%	6.91	6.71	-2.98%
	High price	8.24	8.02	-2.70%	8.29	8.11	-2.18%	7.42	7.23	-2.51%

The annual electricity cost during non-flexible and flexible production in all six scenarios are presented in Table 33. The production of 1081 kt ammonia, 881 kton nitric acid, 479 kt urea, 667 kt urea-ammonium nitrate, and 1028 kt calcium ammonium nitrate cost approximately between 7.3 and 8.3 million euro annually. The findings show that both the increased efficiency as well as the reduced demand scenario, have the highest demand response potential of about 3% cost reduction compared to a non-flexible production process. According to Table 33, producing 8760 hours per year leads the lowest electricity costs during a normal price distribution. Furthermore, an increased production level up to 110% inevitable means that the plants have a broader range between which they can adjust their production speed. As a result, the increased production level scenario tends to be the least sensitive to higher electricity prices with regards to its demand response potential, compared to other two scenarios.

7.5 Blue ammonia scenario

The same six scenarios applied in the BAU scenario are now examined in the blue ammonia scenario, i.e., S2.A.i to S2.C.ii. The hourly electricity consumption and production of ammonia, nitric acid and urea with a normal electricity cost distribution are presented in section 12.2. Due to a substantial increase of electricity required to capture ammonia related CO_2 emissions, fertilizer plants have become much more electricity intensive compared to the BAU Scenario.

Table 34. Electricity costs to produce ammonia, nitric acid and urea in the CCS production scenario

Annual electricity cost [Million Euro}		Increased production (110%)			Increased load hours (8760)			Reduced demand (90%)		
		Non-flexible [M€]	Flexible [M€]	Δcost	Non-flexible [M €]	Flexible [M €]	Δcost	Non-flexible [M €]	Flexible [M €]	Δcost
CCS	Normal price	24.44	23.71	-3.00%	23.93	23.23	-2.93%	22.00	21.33	-3.03%
	High price	26.22	25.50	-2.75%	26.38	25.79	-2.22%	23.60	23.00	-2.56%

Section 12.3 shows that in the 110% production speed scenario, the production speed tends to be either maximum or minimum with less fluctuations compared to the increased load hours and the reduced demand scenario, which is in accordance with the findings of the BAU scenario. The electricity costs and the associated electricity cost savings of flexible production practices in the CCS scenario are presented in Table 34. Although the overall costs increased substantially, approximately the same percentage of electricity cost savings can be achieved in this scenario compared to the BAU. This can be explained by the fact that the process did not change much since the CCS plant only runs when ammonia is produced. As the name already reveals, carbon capture and storage is already a storage process, hence, no additional flexibility potential is introduced in this scenario. Lastly, the increased production scenario tends to be the least sensitive strategy to high electricity prices which leads to the most optimum scenario.

The total electricity costs of a fertilizer production facility in 2030 in the BAU and the CCS scenario are presented in Figure 23. The bar charts of Figure 23 show that the electricity cost of for instance the CCS Flexible production slightly differs for the varying production profile scenarios (e.g., increased production, increased load hours, and reduced demand) and electricity price distributions (e.g., normal, and high price distribution in 2030). Nonetheless, the relation between the CCS non-flexible production and CCS flexible production is for all scenarios quite similar with regards to the electricity cost reduction potential.

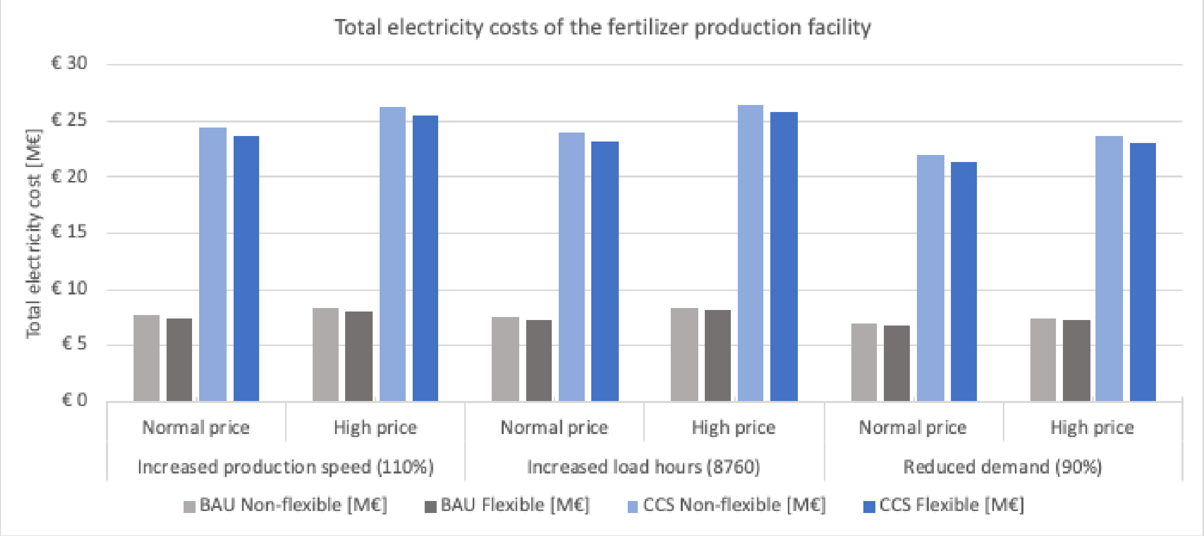


Figure 23. Total electricity costs of a (non-) flexible fertilizer production facility in the BAU and CCS Scenarios with a normal and high electricity price distribution in 2030.

7.6 Green ammonia scenario

In the Green Ammonia scenario, the three strategies to implement flexible production possibilities are again examined to determine which strategy leads to the most optimal production conditions with regards to its balancing properties. The production of all fertilizer (intermediate) products via the Green Ammonia route does not lead to direct CO_2 emissions due to a fully electrified production process. Electrification of the fertilizer production facilities inevitable results in a significant increase of electricity requirement by substituting fossil fuel fired processes. Different from the BAU and the CCS scenario, the Green Ammonia process has an extra production step, i.e., the synthesis of hydrogen in the electrolyzer. The electrolyzer is not bound to a minimum production speed nor a ramp up down rate, hence, fluctuating its output has a significant load shift potential. Moreover, hydrogen produced in the electrolyzer can be stored in a hydrogen storage facility before consumption in the ammonia plant. The hourly fertilizer production speed with the associated electricity consumption profile of all three strategies are represented in section 12.3.

Section 12.3 provides a clear visualization of the important role of the electrolyzer with a hydrogen storage tank on its loads shifting potential. The graph of the electrolyzer production output in combination with state of the hydrogen storage, shows how fluctuations in electricity prices can be balanced out. Moreover, the electricity cost savings in the Green Ammonia scenario are higher compared to the other two scenarios, as shown in Table 35.

Table 35. Electricity cost for the production of ammonia, nitric acid and urea in the Green Ammonia scenario

Annual electricity cost [Million Euro}		Increased production (110%)			Increased load hours (8760)			Reduced demand (90%)		
		Non-flexible [M€]	Flexible [M€]	Δcost	Non-flexible [M €]	Flexible [M €]	Δcost	Non-flexible [M €]	Flexible [M €]	Δcost
Green Ammonia	Normal price	704.1	678.7	-3.6%	689.3	664.9	-3.5%	635.9	610.1	-4.1%
	High price	755.4	725.1	-4.0%	759.9	733.5	-3.5%	682.2	652.9	-4.3%

Contrarily, in the Green Ammonia scenario, the demand response potential of the integrated production facility becomes larger during a high electricity price distribution compared to a normal electricity price distribution. The highest electricity costs savings are achieved when implementing the increased efficiency scenario during high electricity prices, as shown in Figure 24.

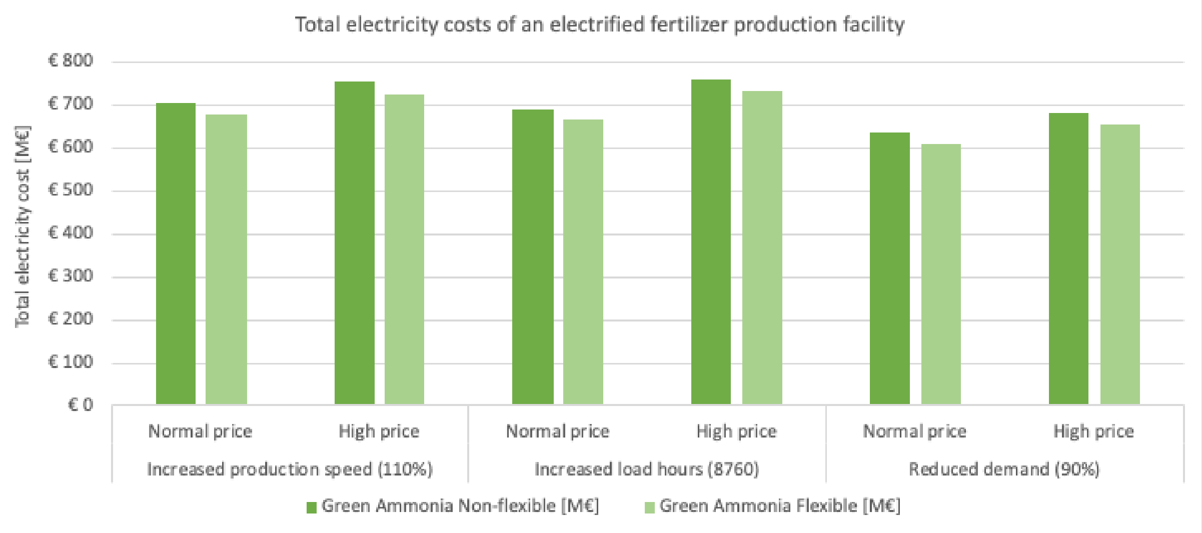
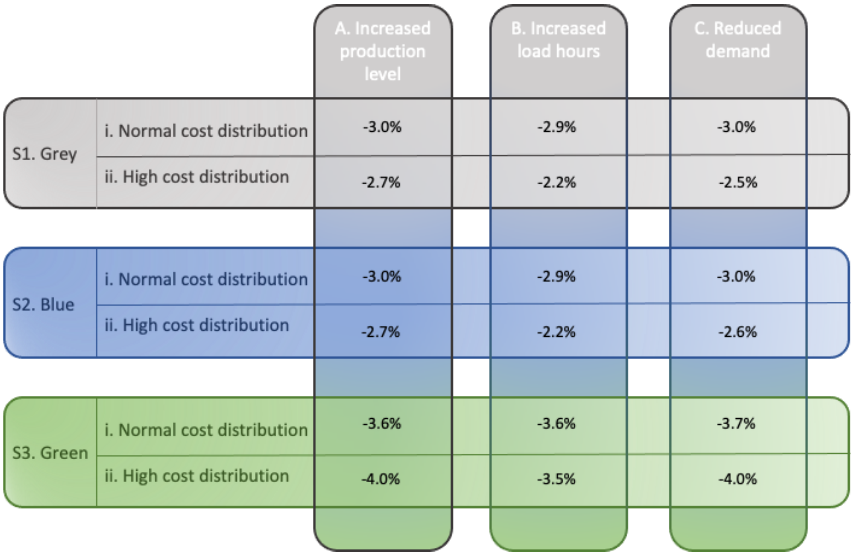


Figure 24. Total electricity cost of fully electrified fertilizer production facility Green Ammonia Scenario with a normal and high electricity price distribution in 2030.

7.7 Comparison

The total electricity cost reduction of all 18 scenarios, are presented in Figure 25. The grey and blue scenarios show a trend where the net cost reduction caused be flexible production is relatively lower during high electricity prices with more outliers compared to a normal electricity price distribution. Contrarily, in the green electrified production process scenarios, the relative electricity cost reduction tends to be higher during high electricity prices compared to a normal price distribution. This could be explained by the increased flexibility of operation in the Green Ammonia scenario due to the electrolyzer. A more flexible production process is more effective in avoiding high price peaks. Notably, the relative cost reduction as presented in Figure 25 only displays the potential electricity cost reduction of a potential flexible production profile in the associated production scenario.



		A. Increased production level	B. Increased load hours	C. Reduced demand
S1. Grey	i. Normal cost distribution	-3.0%	-2.9%	-3.0%
	ii. High cost distribution	-2.7%	-2.2%	-2.5%
S2. Blue	i. Normal cost distribution	-3.0%	-2.9%	-3.0%
	ii. High cost distribution	-2.7%	-2.2%	-2.6%
S3. Green	i. Normal cost distribution	-3.6%	-3.6%	-3.7%
	ii. High cost distribution	-4.0%	-3.5%	-4.0%

Figure 25. Relative electricity cost savings potential of all 18 scenarios compared to a non-flexible production profile

Although Figure 25 implies that the cost savings are somewhat similar for all 18 scenarios, the absolute electricity cost savings differ in 2 magnitudes of order (i.e., €0.23 M in S1.A.i compared to €25.4 M in S3.A.i) due to a substantially higher share of electricity consumption in the Green Ammonia scenario, as shown in Figure 26. Therefore, only the values in the Green Ammonia Scenario present an accurate demand response potential of the proposed production scenario. In the BAU and CCS scenario, on the other hand, besides electricity also natural gas is consumed during the production process of ammonia. In addition, both the BAU and the CCS scenario led to greenhouse gas emissions. Therefore, the projected natural gas price and carbon pricing strategy in 2030 had to be considered.

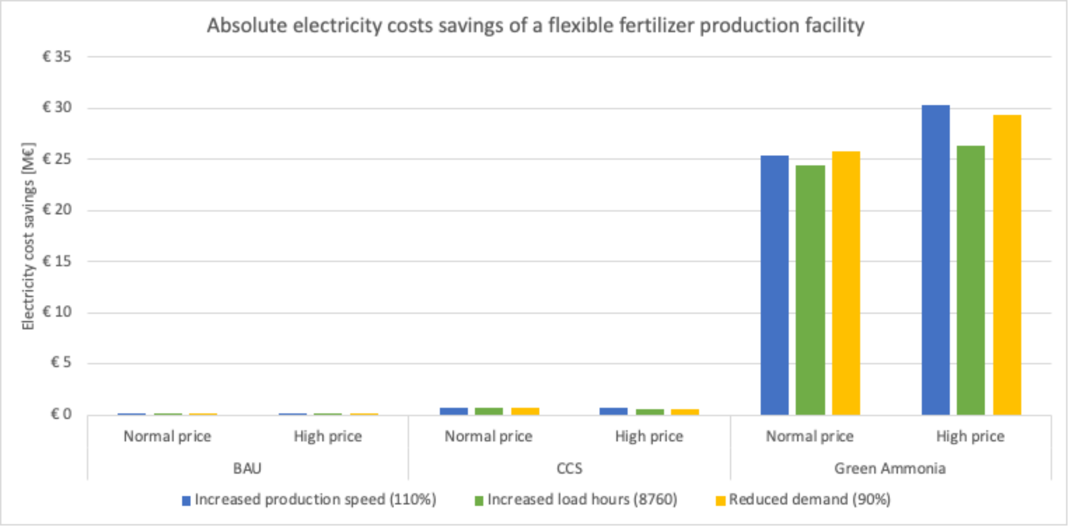


Figure 26. Absolute electricity cost savings of a demand response application in a flexible fertilizer production plant in for all 18 scenarios described in Figure 19.

The energy cost per tonne of ammonia produced are calculated for a natural gas price equal to the average 2021 – 2022 level (€90 per MWh (Sönnichsen, 2022b)), carbon price of €120 by 2030 as projected by the United Nations (UN-Convened Net-Zero Asset Owner Alliance, 2021) and electricity prices for the Netherlands from the MIX-2030 simulation and presented Figure 27. Figure 27 visualizes the relative cost reduction of a flexible production profile for S1.A.i, S2.A.i, and S3.A.i. These scenarios were chosen since the 110% production level is considered the most realistic scenario as it is based on the adaptivity of a production plant according to its design characteristics. Moreover, the relative cost reduction differences between for instance all scenarios from the S1 category could be considered negligible.

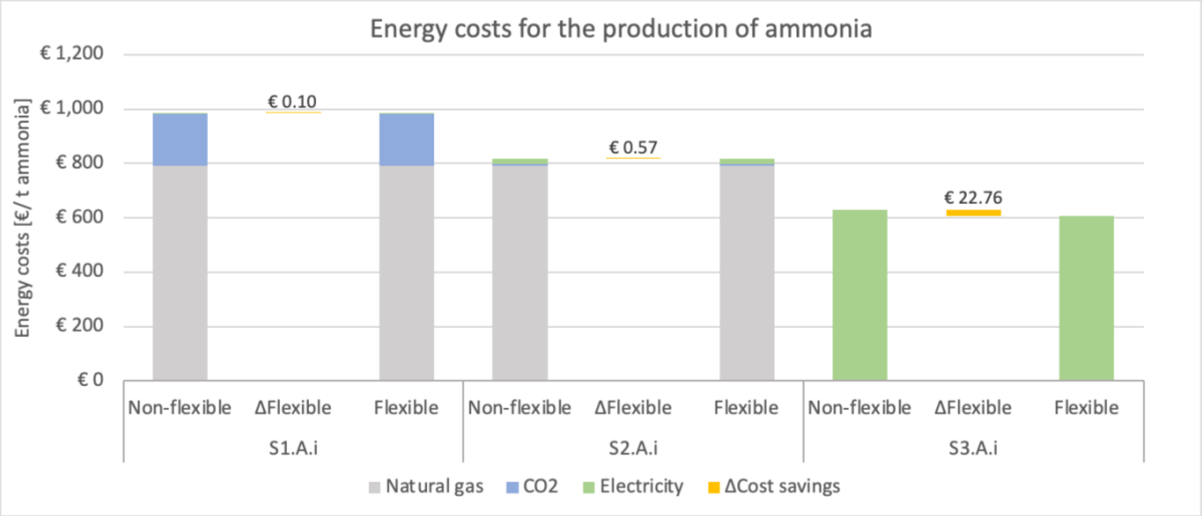


Figure 27. Energy costs to produce ammonia in S1.A.i, S2.A.i, and S3.A.i with both a flexible and a non-flexible production profile. Assuming that by 2030 natural gas costs €90 per MWh and a carbon pricing of €120 per tonne CO_2 emitted.

Figure 27 shows that the cost savings potential in non-fully electrified production processes is negligible, i.e., 0.01% and 0.07% per tonne ammonia for S1.A.i and S2.A.i respectively. Moreover, the absolute cost reduction potential of a flexible production profile in these two scenarios is predominantly determined by the price of natural gas and the associated total natural gas costs., Adapting to flexible production possibilities could potentially be more cost intensive than its savings potential. For the fully electrified production process, a flexible production profile could potentially reduce the total energy costs to produce one tonne ammonia by 3.6% resulting in €22.7 per tonne ammonia. Ultimately, considering the S3.A.i scenario, the economic demand response potential of fully electrified fertilizer production facility by 2030 is approximately €25.4 million resulting in 3.6% total energy cost reduction. Subsequently, based on the economic demand response potential of S3.A.i., the associated technical demand response potential is determined. A flexible production profile of the ammonia, nitric acid, urea, and electrolyzer lead to a load shifting effect on the grid. Figure 28 presents a visualization of the load shifting potential of the ammonia, nitric acid, and urea plant.

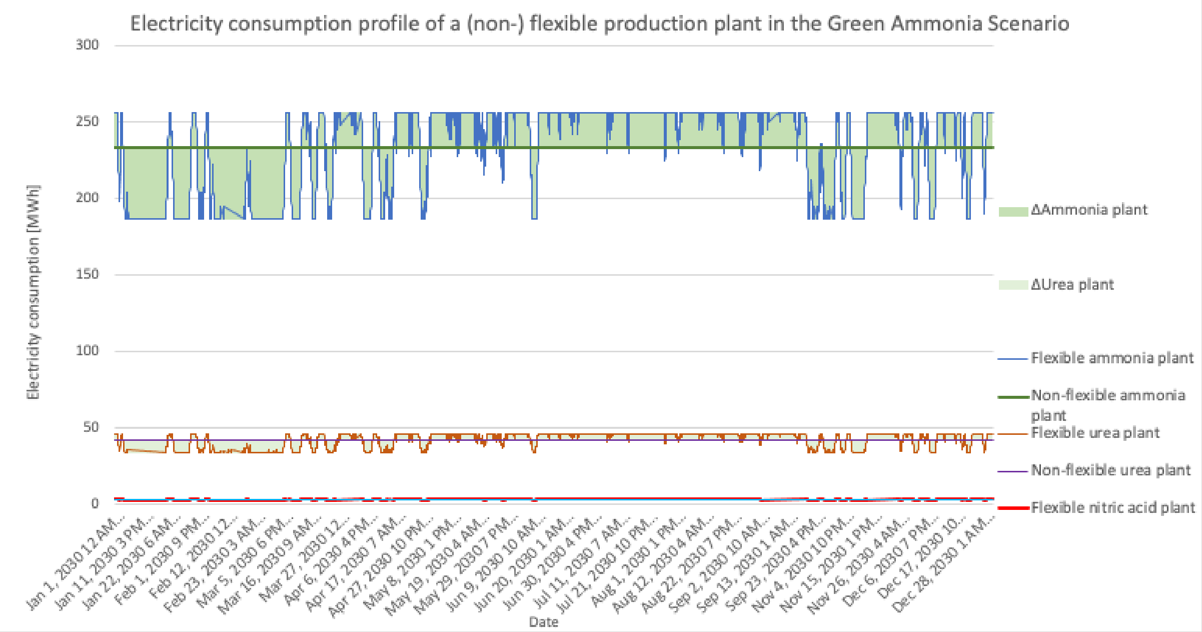


Figure 28. Electricity consumption profiles of (non-) flexible fertilizer production plant in the Green Ammonia scenario (S3.A.i)

Since the electrolyzer has no technical constraints with regards to the ramp up/ down rate, visualizing a flexible electrolyzer production plant does not clearly show its load shift potential, hence, electricity consumption in the electrolyzer is excluded from Figure 28 and presented in section 12.3. Differences between the flexible and the non-flexible production profile of the electrolyzer, ammonia, nitric acid, and urea plant determine the technical demand response potential of a fully electrified European nitrogenous fertilizer production plant in 2030. The specific technical demand potential of the four plants is presented in Table 36. The findings show that the ammonia, nitric acid, and urea plant have a similar load shifting potential in terms of percentage, whereas the electrolyzer has a 6.5 percentage points higher peak shifting potential. Ultimately, an electrified fertilizer production facility has a technical demand response potential of 16.6% leading to 1,898 GWh peak shifting per year.

Table 36. Technical demand response potential of a flexible fertilizer production plant in the Green Ammonia scenario (S3.A.i)

Technical demand response potential	Electricity consumption [GWh/year]	Load shift potential [GWh/year]	Percentage
Electrolyzer	9,191	1,646	17.9%
Ammonia plant	1,862	212	11.4%
Nitric acid plant	24	3	11.2%
Urea plant	333	38	11.3%
Total	11,411	1,898	16.6%

8 Discussion

In this section, all points of discussion related to the research are pointed out to draw a conclusion from the results and to see where future research should focus at. The discussion is divided into two sections. At first, the results are discussed in three subsections: consumption and production profile estimations, cost estimations, and demand response potential. Second, a sensitivity analysis is conducted to determine the impact of the input parameters of the optimization model on the output.

8.1 Discussion of results

Consumption and production profile estimations

The research started by estimating the current energy consumption profile of OCI Nitrogen's and Yara Sluiskil's integrated nitrogenous fertilizer production facilities and their associated greenhouse gas emissions in chapter 4. These estimations where predominantly based on published energy consumption profiles of OCI's and Yara's ammonia, nitric acid, urea plants (Batool & Wetzels, 2019). Unfortunately, during a personal interview with the Sustainability Manager of OCI Nitrogen they concluded that more detailed numbers of their energy consumption profile would be impossible due to confidentiality reasons. In addition, the Head of Environmental Care of Yara Sluiskil was initially willing to share absolute numbers of company data related to energy consumption profiles of the production plant. However, they decided that sharing this data was confidential, hence, that this research is based on figures published in (Batool & Wetzels, 2019). In combination with lacking literature, the assumption is made that the ammonium nitrate, urea ammonium nitrate, and calcium ammonium nitrate plants do not require energy input, thus, in the decarbonization scenarios, they are not considered when estimating alterations in the energy consumption profiles of the production plants. However, substituting the primary and secondary steam methane reactors in the Green Ammonia Scenario could probably alter the integrated heat system from the ammonia plant to the other plants. Therefore, this research examines the demand response potential of a somewhat simplified fictive integrated fertilizer production facility.

Regardless of the ammonia production route, the production of 1 tonne urea requires 0.73 tonne CO_2 as feedstock (Kool et al., 2012). Since fertilization with urea also leads to an increased carbon concentration in the soil, the amount of CO_2 released upon spreading could be considered lower than direct emissions during combustion. Although fertilizer companies do not include the consumption of CO_2 in their annual sustainability reports, soil fertilization with urea or urea ammonium nitrate results in the release of the CO_2 stocked in the product (European Commission, 2007). On the other hand, some scholars consider CO_2 input for urea production a carbon capture and utilization potential (Driver et al., 2019). Driver et al. (2019) state that green ammonia with CO_2 in another industrial process leads to 'Blue Urea" with a reduced environmental impact compared to conventional urea. Moreover, Driver et al. (2019) consider the production of blue urea carbon neutral. Other scholars would disagree with their findings as sustainable fertilizer production should aim at carbon free fertilizer production requiring a shift away from urea containing fertilizer production (Gielen et al., 2022). This research did not include the potential of carbon capture and utilization by integrating the CCS system with the urea production plant. In fact, the cost of CO_2 consumption where not taken into consideration. Further research should quantify the indirect CO_2 emissions of urea fertilization and determine whether sustainable fertilizer application should shift away from carbon containing fertilizer products.

Substituting conventional steam methane reformer reactors requires an alternative hydrogen source to form NH_3 from N_2. In the green ammonia scenario, a large electrolyzer will produce this hydrogen with electricity as the energy source. The electrolyzer used in the flexible production estimation in chapter 5 requires an installed capacity of around 1.3 GW. Recently, Shell announced that they started with the construction of the first green hydrogen production facility in the Rotterdam harbor area

(Koster, 2022). This new hydrogen production facility should be ready in 2025 and have the largest capacity so far worldwide of 200 MW. Based on this new project, another facility will be developed in Delftzijl with an approximate capacity of 1 GW by 2030. Therefore, a completely electrified nitrogen fertilizer production facility in 2030 could be unrealistic. Furthermore, this research assumes that the production of 1 kg hydrogen requires 47 kWh. However, Ikäheimo et al. (2018) projected that a PEM electrolyzer will have a specific electricity consumption of 44 – 53 kWh per kg ammonia. Building an electrolyzer with higher efficiency than assumed in this research could reduce the required capacity significantly. Further research should examine the feasibility of a green ammonia production plant with the size of a conventional grey ammonia plant.

Cost estimations

In chapter 6, the marginal production cost of ammonia is estimated for all three scenarios with a varying natural gas price and CO_2 emission prices. The paper of Ikäheimo et al. (2018) estimated the production cost of 1 tonne of ammonia at around €430/t NH_3 considering a natural gas price of 46 €/MWh. In this research, the production of 1 tonne ammonia with a natural gas price of €46/MWh is around €406. This could be explained by the difference in estimated natural gas consumption per tonne ammonia of 35.6 GJ by Ikäheimo et al. (2018) and 31.8 GJ /t NH_3 in this research. If CO_2 emissions are not considered, Ikäheimo et al. (2018) estimated that natural gas prices should exceed €70/MWh to make a power-to-ammonia production route become competitive to methane-fed ammonia production. This research estimated that the CCS production route would become profitable when natural gas prices exceed €69/MWh. Ultimately, these findings are somewhat in line with existing literature on power-to-ammonia possibilities. Nonetheless, this research assumed that the future natural gas price will be €90/MWh which could be considered a limitation since existing research lacks projections of future natural gas price development. In the REPowerEU Plan the European Commission presents its response to the global energy market disruption which is predominantly caused by Russia’s invasion in Ukraine. The REPowerEU Plan aims at ending the EU’s dependence on fossil fuels from Russia due to economic, political, and environmental motives (European Commission, 2022). Measures like energy savings, diversification of energy supplies, and accelerated roll-out of renewable energy will become of great importance to reach its goal and to replace fossil fuels in homes, industry, and power generation. One could say that despite current extreme fluctuating natural gas prices due to geopolitical conflicts, the natural gas price assumption is hard to justify. However, the REPowerEU Plan aims at reducing fossil fuel consumption in industry by supporting the uptake of green hydrogen to substitute natural gas (European Commission, 2022). Ultimately, further research should examine more realistic projections of natural gas price development.

Demand response potential

The optimization model showed that flexible low-carbon fertilizer production facilities could potentially reduce the overall electricity cost per tonne of product. Despite the assumption that the production plants are constraint by a minimum and maximum production speed, flexible production inevitably leads to a flexible supply of products. This would require a paradigm shift in the current market with regards to a matching demand and supply. Another option could be that current storage facilities function as a buffer to match the demand with a varying supply. Further research should therefore focus on the current demand and supply of fertilizer products to examine the impact of flexible production on the annual supply of final products and determine whether a flexible production profile could lead to mismatches on the nitrogenous fertilizer market.

Appendix 1 to 3 show that the ammonia storage capacity of 33 kt is more than ten times bigger in size than the range between the minimum and maximum storage level during the simulation. As result, to facilitate flexible production properties to nitrogenous fertilizer plants, storage capacities are allowed to be much lower than 10% of the estimated production of final products annually. Moreover, an assumed installed hydrogen storage capacity of 5.8 kt is around twice the size of the current installed underground storage facilities in the Clemens and Moss Bluff salt caverns. Furthermore, this research does not include investment costs and energy requirements for the storage of chemical products. There is assumed that hydrogen will be stored underground since liquified hydrogen storage is more capital and energy intensive. However, the report of Davies et al. (2020) state that with large scale hydrogen plants (> 50 tonnes/ day) the energy requirements and the associated investment (CAPEX) and operation costs (OPEX) could be halved compared to current operational hydrogen liquefaction plants. Ultimately, to get a more accurate estimation of the electricity costs per ton of product and the association cost reduction potential of DR application, the energy requirements of storage tanks should be included.

8.2 Sensitivity analysis

Since both the BAU and CCS scenario consume natural gas as the main energy source, flexible production results in low total energy cost reduction (between 0.1% and 0.6%). Therefore, the sensitivity analysis is only performed on the Green Ammonia Scenario by varying multiple input parameters that determined the demand response potential. The increased production speed level to 110% is considered more realistic than increased load hours annually or a year with a reduced demand because no adjustments are needed to implement this scenario in existing fertilizer production plants. Therefore, scenario S3.A.i is used as the reference scenario for the sensitivity analysis. Additionally, the sensitivity analysis is conducted with a normal electricity price distribution of the MIX-2030 scenario of the electricity price simulation. The changed input parameters of the sensitivity analysis are described in Table 37.

Table 37. Sensitivity analysis of the optimized Green Ammonia Scenario.

Input parameters		Description
Green ammonia	**Reference scenario (S3.A.i)**	Scenario S3.A.i refers to a scenario of Figure 16. In this scenario the min production speed is set at 80%, max at 110% with 8000 load hors annually and a normal price distribution of electricity cost.
	1. Min production speed	The minimum production speed level is altered from 80% in reference scenario to 70% and 90% for the ammonia, nitric acid, and urea plant
	2. Max production speed	The maximum production speed is altered from 110% in reference scenario to 105% and 115% for the ammonia, nitric acid and urea plant, and the electrolyzer.
	3. Ramp up/down rate	The ramp up/ down rate of the ammonia, nitric acid, and urea plant are altered from 1.25% per hour to a 4 times smaller and 4 times larger rate, i.e., 0.31% and 5% per hour
	4. Electrolyzer capacity	Only the installed capacity of the electrolyzer is altered from 110% in reference scenario to 105% and 115%.
	5. Hydrogen storage	The hydrogen storage capacity is altered from 100% in the reference scenario to 50% and 150%.
	6. Electrolyzer capacity and hydrogen storage	The installed capacity of the electrolyzer is altered from 110% in reference scenario to 105% and 115% and the hydrogen storage capacity is altered from 100% in the reference scenario to 50% and 150% simultaneously.
	7. Oversized electrolyzer	Only the installed capacity of the electrolyzer is oversized from 110% in reference scenario to 130%
	8. No technical constraints	In this scenario, limiting constraints like the ramp up/ down rate and a minimum production level for the ammonia, nitric acid, and urea plant are left out.

At first, the simulation considered a maximum production level of 110% based on the Chemical Engineer Design characteristics of Sinnot (2005) and a minimum production level of 80% based on personal communication with OCI Nitrogen. OCI Nitrogen mentioned that the production speed should never be lower than 70% but that 80% would be preferable. A minimum and maximum production speed of 70% and 110% respectively is somewhat in line with the paper of research of Armijo & Philibert (2020) who examined flexible production of ammonia with a range in production speed of 60% to 105%. The sensitivity analysis shows that changing the minimum production speed parameters by ± 10 percentage points only slightly effects the reduction potential, Figure 29.

Secondly, Coulson and Richardson (2005) posed that average production equipment is generally oversized by 10% to ensure a safe plant design. This research examines the demand response potential of a fictive fertilizer production plant by 2030. Therefore, this fictive plant must be designed before the implementation of flexible production possibilities. One could therefore question why a new fertilizer plant will not be oversized by 15% to lubricate the flexibility of operation. The impact of such a size increase is presented in Figure 29. Ultimately, oversizing the ammonia, nitric acid, urea plants and the electrolyzer by ± 5 percentage points does have a major impact on production cost reduction potential, as shown in Figure 29. Notably increasing the max production by 5 percentage points has a larger impact on the cost reduction potential than decreasing the min production level by 10 percentage points

Thirdly, to integrate flexible production possibilities in a production plant, the plant should be able to ramp up or down its production speed. For the optimization model there was assumed that increasing or decreasing the production speed by 5% takes approximately four hours. However, in the flexibility analysis of a Haber-Bosch ammonia production plant of Armijo & Philibert (2020) the production speed could be ramped up or down with 20% per hour. Since their research set up is almost 100 times smaller in size, the ramp up and down rate per hour is multiplied and divided by 4 to determine its effect on the flexibility potential. Figure 29 shows that varying ramp up and down rate parameters results in a negligible DR potential change

At fourth, a decrease of the minimum production level of the ammonia, ammonium nitrate and urea production plant resulted in just a slight increase of reduction potential of 0.17 percentage point. To determine whether the significant increase of the reduction potential during an increased production speed level is caused by the increased electrolyzer capacity or by the ammonia, nitric acid, and urea plant, the cost reduction potential is also simulated for just an increased electrolyzer capacity (105% and 115%) cetris paribus, as presented in Figure 29. The findings shows that the 1.39 percentage points increase of the cost reduction potential of the increased production speed level is for 1.12 percentage points caused by the electrolyzer and only 0.27 percentage points related to the ammonia, nitric acid, and urea plants.

At fifth, the installed hydrogen storage capacity is estimated by using the same ratio of the storage capacity of ammonia compared to the annual production of ammonia. This has led to an installed hydrogen storage capacity of 5 kt. A green hydrogen production facility with an underground hydrogen storage capacity in France's Ain region has a daily production estimate of 400 kg hydrogen and a storage capacity of 3 tonnes. When converting this ratio to the fictive green ammonia production plant of this research leads to a hydrogen storage capacity of 4.3 kt and an hourly production of 23 tonnes green hydrogen. This would mean that the assumption of 5.8 kt is slightly higher but still reasonable. However, due to the size of this facility, the sensitivity analysis examines the effect of increasing and decreasing the storage capacity by 50%. According to Figure 29, the assumptions made for the estimations of the storage capacity do not significantly affect the DR potential.

At sixth, the fourth and fifth scenario are combined to determine whether the impact of an increase in electrolyzer capacity on the reduction potential is limited by a constant hydrogen storage capacity and vice versa, both the electrolyzer capacity and the hydrogen storage capacity are increased or decreased accordingly. Figure 29**Error! Reference source not found.** shows that a combined alteration of these parameters leads to a reduction potential equal to the sum of both parameters altered separately. Therefore, under these fertilizer plant conditions, the electrolyzer capacity is not limited by the hydrogen storage capacity and vice versa.

At seventh, altering input parameter 2, 4, and 6 showed that maximizing the cost reduction potential predominately depends on the size of the electrolyzer. This is in line with the findings of (Bruns et al., 2022) who stated that oversizing the electrolyzer can reduce the operating costs (OPEX) inevitable leading to an increase of the investment costs (CAPEX). Increased investment costs lead to higher hydrogen production costs. However, existing literature lacks knowledge on the optimal magnitude of oversizing an electrolyzer to lubricate demand response applications. Therefore, future research should examine the trade-off between an improved flexibility of operation leading to a decreased OPEX and the associated increased CAPEX. The research of Vogl et al. (2018) on fossil-free steelmaking processes increased their flexibility of operation by oversizing the electrolyzer by 30%. Figure 29 shows that an electrolyzer 30% larger than required leads to almost doubled electricity cost reduction from €25.4M reduction to €48.9M cost reduction annually. This additional €23.5M electricity cost reduction leads to an inevitable CAPEX increase since such an electrolyzer requires an installed capacity of 1.49 GW instead of 1.26 GW. Further research should determine whether oversizing an electrolyzer by 30% is financially worth it.

Lastly, according to above presented results, decreasing the current minimum production speed level by 10%, multiply the ramp up rate by 4, or reduce the existing hydrogen storage capacity half in size happens to have only a slide impact on the overall production cost reduction. Moreover, there could be concluded that oversizing a production facility seems to have the highest potential to reduce the overall production cost by implementing flexible production strategies. However, to see how current input parameters constraint to system, the potential cost reduction is determined for the S3.A.i scenario where no constraints are in place, i.e., the production speed level is limited by 110% but the production profile is not limited by a minimum production speed nor a ramp up/ down rate. Figure 29 shows that the minimum production speed level and the ramp up/down rate parameters slightly constraint the model as they reduce the reduction cost potential by 0.59 percentage points.

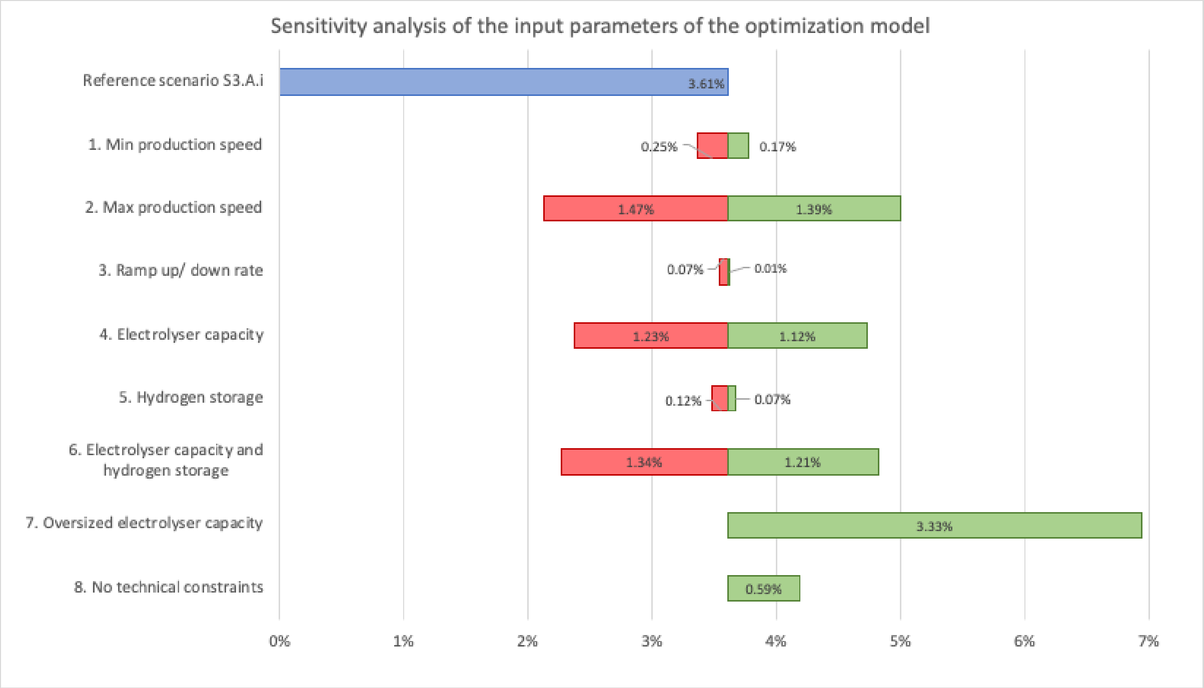


Figure 29. Results of sensitivity analysis.

9 Conclusion

The fertilizer industry is a high energy intensive industry requiring 2 – 3% of the global energy consumption. Nitrogenous fertilizer products predominantly depend on the input of natural gas as a fuel and feedstock to produce ammonia form atmospheric nitrogen and methane. With nitrogenous fertilizers being the vast majority globally, nitrogenous fertilizer production facilities will seek some major endeavors with regards to soaring natural gas prices and a global movement towards a higher share of sustainable energy in the fuel mix to meet the carbon neutrality goals set by the United Nations. This research aims at estimating the demand response potential of a low carbon fertilizer production facility in 2030. To move towards a more sustainable production route for fertilizer products, existing energy consumption profiles of fertilizer production facilities are examined and quantified. The production of ammonia is considered the energy intensive production step of fertilizer production facilities. Many conventional ammonia plants are methane-fed production routes. The analysis of OCI Nitrogen and Yara Sluiskil showed that both companies have quite a similar energy consumption, fertilizer production, and greenhouse gas emission profile operating for 8000 hours per year. The energy consumption profiles showed that in fertilizer production facilities electricity is consumed in the ammonia, nitric acid, and urea plant.

Following, the examination of the energy production profiles of three decarbonization scenarios (i.e., BAU, CCS and Green Ammonia) have shown that the BAU and CCS scenario are still predominantly reliant on natural gas. In the BAU, projections of the Best Available Technology in 2030 are implemented which resulted in a 10% natural gas consumption reduction compared to existing profile of OCI Nitrogen. In addition, only 1.3% of the total energy consumption of a production facility is electricity. Although the implementation of a CCS system significantly increases the electricity consumption by more than a three-fold, it is still only a 3% increase of the total energy consumption while 96% of the CO_2 emissions will be captured and stored. In the Green Ammonia Scenario, the total final energy requirements increased by approximately 15% without the side effect of CO_2 emissions since the production process is completely electrified. A fully electrified fertilizer production facility is estimated to consume 11.4 TWh electricity per year by 2030 which accounts for an approximate increase of 9000% and 3000% electricity consumption increase compared to the BAU and CCS scenario respectively. Considering an average annual electricity consumption of 2,730 kWh per household in the Netherlands in 2019 (CBS, 2021), a fully electrified fertilizer production facility requires the same amount of electricity as 4.2 million dwellings.

Following, the energy consumption profile is compared to the expected price of energy sources. Due to geopolitical conflicts, projection of future trends of carbon pricing and natural gas prices are hard to estimate. Considering electricity prices of MIX-2030 scenario, an implemented carbon pricing strategy of €120/ t CO_2, the Green Ammonia production route is lower in total energy and CO_2 permit costs compared the BAU and CCS Scenario if natural gas prices exceed €49.6 and €69.0 per MWh respectively. If natural gas prices continue to be €90/MWh, an electrified production facility could reduce the total annual energy cost by 34% and 21% per year compared to the BAU and CCS scenario respectively.

For all three fertilizer production routes, flexibility within the production processes were determined and technical constraints defined. Electricity costs were minimized by shifting the production in the three scenarios at times of lower electricity prices, based on hourly electricity price data of two MIX-2030 simulation. Three technical constraining scenarios were developed to include different forms of flexibility to the production facility: 1) increased production speed (110%), 2) increased load hours (8760), and 3) reduced demand (90%). Following, the optimization model was solved for 18 scenarios, a matrix of BAU, CCS and Green Ammonia versus three technical constraining scenarios simulated for two electricity price distributions. The results of these scenarios showed that for all 18 scenarios the total electricity costs could be reduced by 2 to 4 percent. However, since the share of electricity consumed in the BAU and CCS production route was around 1% and 3% respectively, the overall energy cost reduction potential in all the BAU and CCS scenario were close to zero percent. On the other hand, in the Green Ammonia Scenarios the potential electricity cost saving was around 3.6% resulting in €25.4 million electricity cost reduction per year. This cost savings was achieved by shifting in time 1898 GWh per year, corresponding to the 16.6% of the load (i.e., technical demand response potential). Ultimately, the production cost of ammonia was still significantly higher than the prices of ammonia over the last decade. However, compared to the last year’s average, renewable electricity fed ammonia production could be a viable option for hydrogen supply to nitrogen fertilizer production plants, enabling the decarbonization of this highly energy intensive and CO_2 emitting industrial sector.

Based on the sensitivity analysis, the conclusion can be drawn the demand response potential is predominantly limited by the flexibility of operation of the production process and the range of the electricity price distribution. The economic demand response potential increases during times of stronger fluctuating day-ahead electricity prices. For the ammonia, nitric acid, and urea plants, increasing ranges between minimum and maximum production speeds, increased ramp up/ down rate and installed storage capacity only slightly improved the flexibility of operation. The size of the electrolyzer showed to have the biggest impact on the flexibility of operation. As a result, the technical demand response potential and, inevitably, the associated economic demand response potential could be increased by oversizing the electrolyzer up to a point where the additional CAPEX and OPEX of an oversized electrolyzer are still lower than the annual electricity costs reduction caused by demand response applications.

Ultimately, the demand response potential of a low carbon fertilizer production facility in 2030 depends on the share of electricity in the total energy consumption profile of the facility. For grey and blue ammonia production routes, the amount of electricity is too low to implement flexible production processes to achieve a substantial electricity cost reduction. Concerning a green hydrogen fed ammonia production route, flexible production activities could reduce the total energy costs by 3.6% resulting in a load-shifting potential of more than 16%. Therefore, a low carbon flexible fertilizer production facility could financially benefit from a flexible production profile while enhancing grid balancing.

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0&resolution.values=PT15M&resolution.values=PT30M&resolution.values=PT60M&dateTime.timezone=CET_CEST&dateTime.timezone_input=CET+(UTC+1)+/+CEST+(UTC+2)

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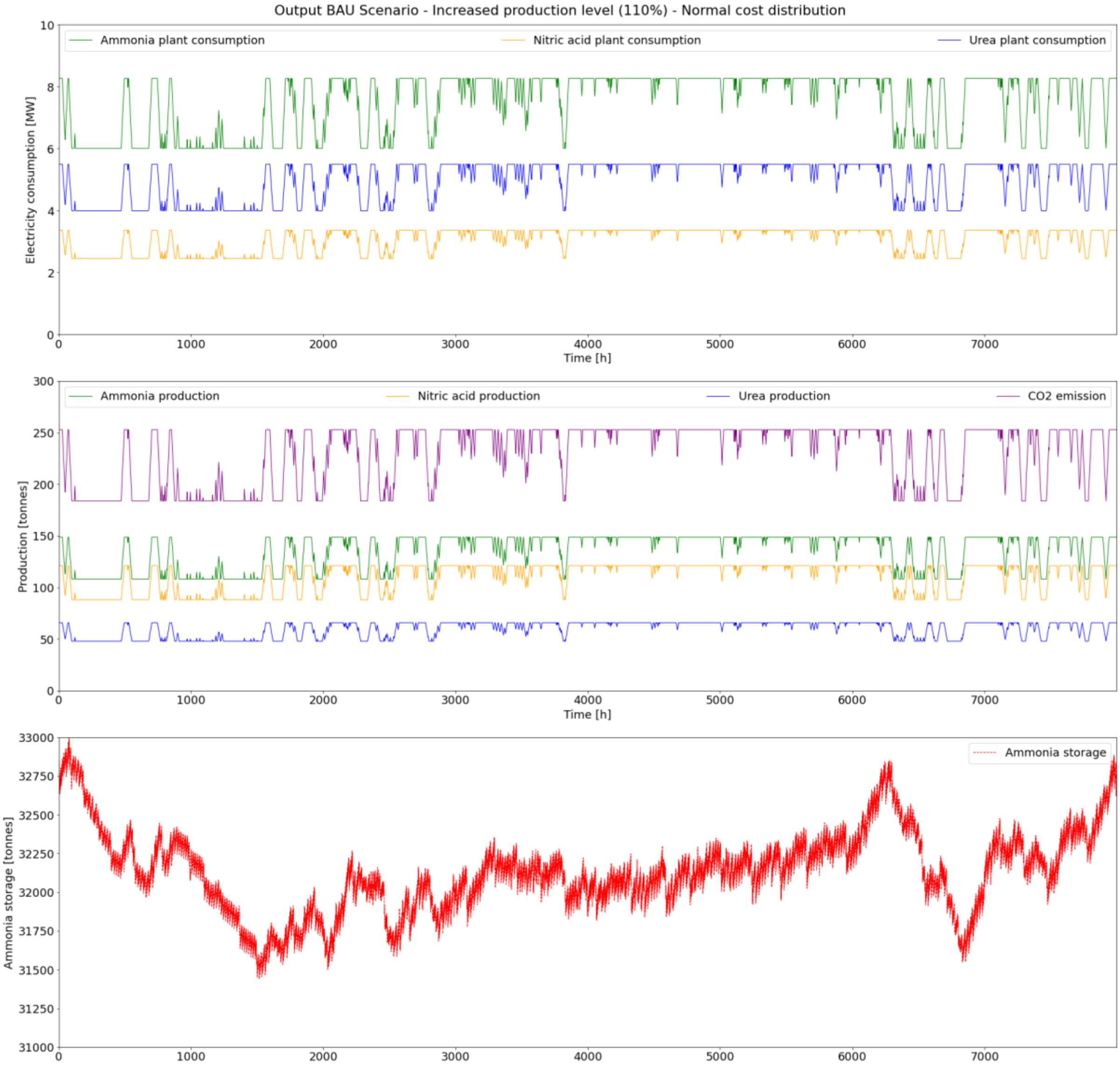
12 Appendix

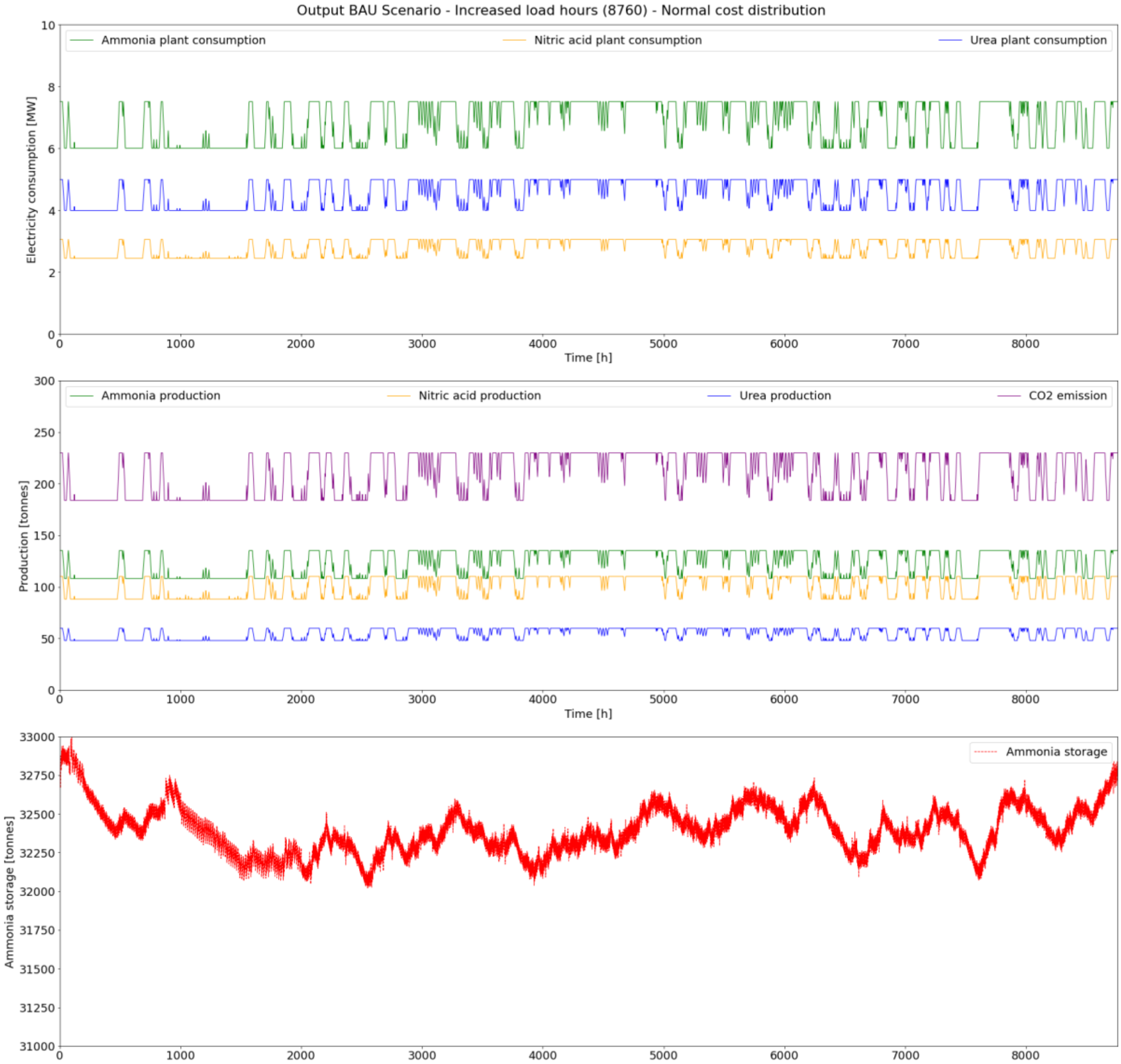
12.1 Appendix 1 BAU simulations

1.1 Simulation output BAU Scenario with Normal cost distribution

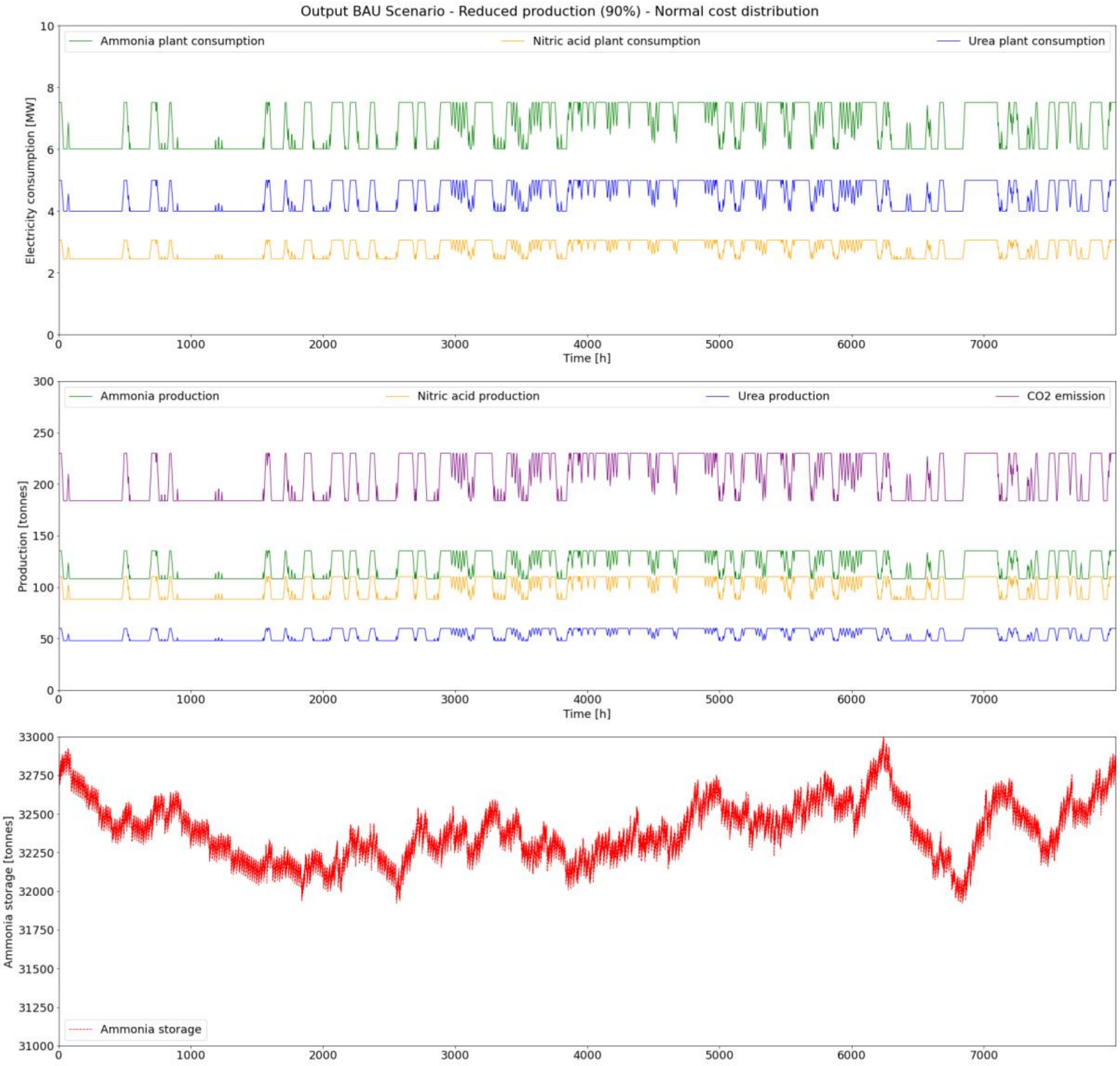
S1.A.i



S1.B.i

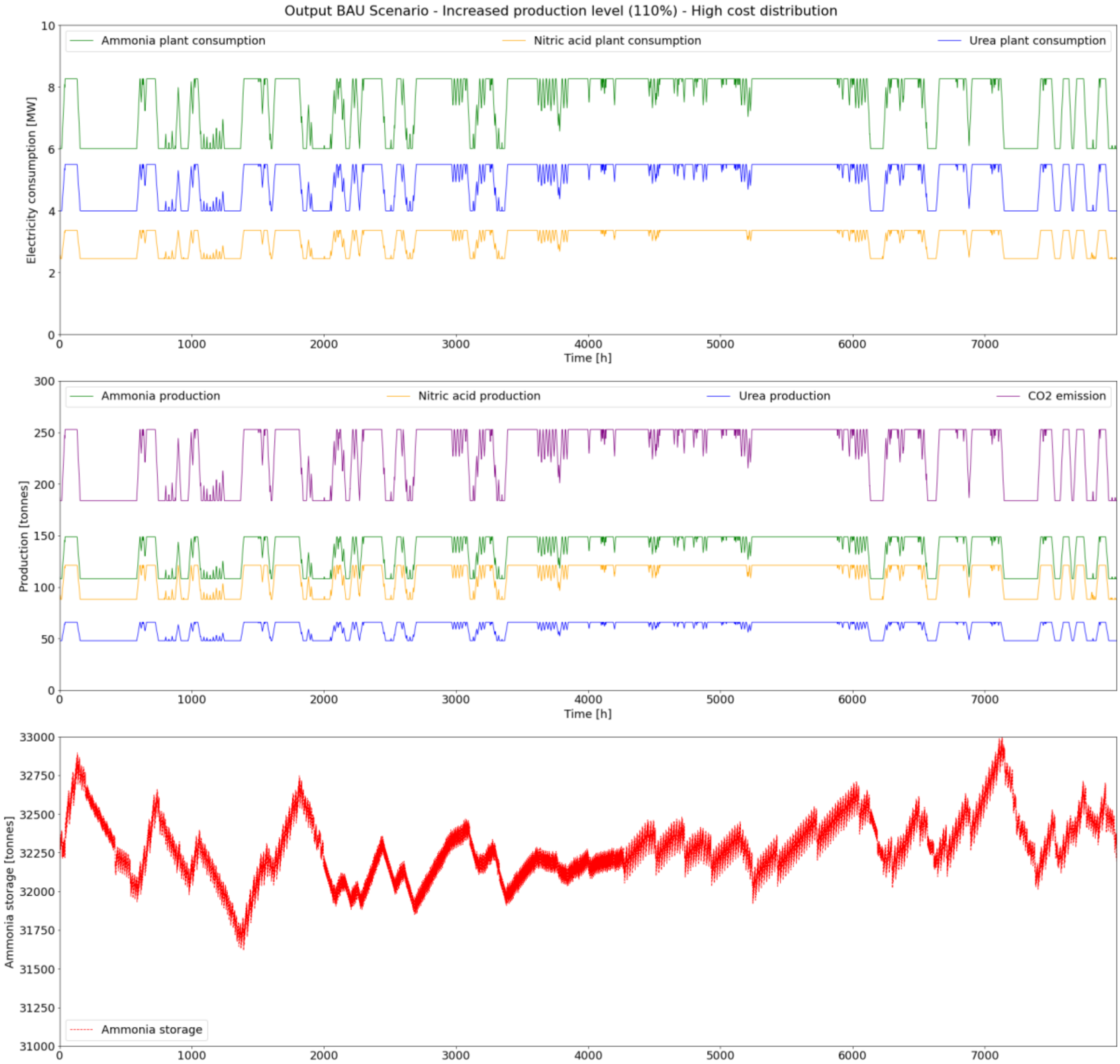

Output BAU Scenario - Increased load hours (8760) - Normal cost distribution
Ammonia plant consumption
Nitric acid plant consumption
Urea plant consumption
Electricity consumption [MW]
0
2
4
6
8
10
0
1000
2000
3000
4000
5000
6000
7000
8000
Time [h]
Ammonia production
Nitric acid production
Urea production
CO2 emission
Production [tonnes]
0
50
100
150
200
250
300
0
1000
2000
3000
4000
5000
6000
7000
8000
Time [h]
Ammonia storage
Ammonia storage [tonnes]
31000
31250
31500
31750
32000
32250
32500
32750
33000
0
1000
2000
3000
4000
5000
6000
7000
8000

S1.C.i

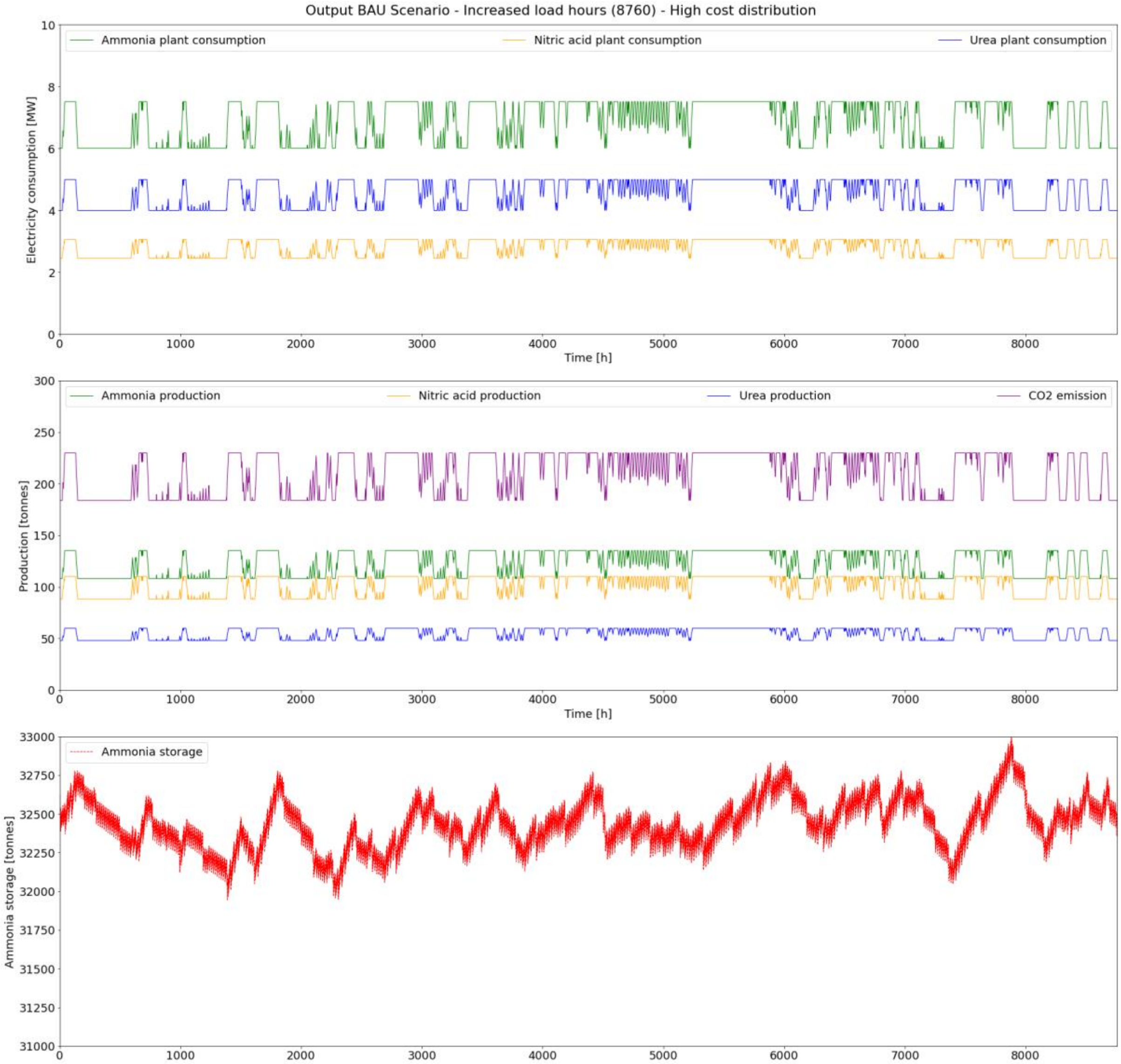

Output BAU Scenario - Reduced production (90%) - Normal cost distribution
Ammonia plant consumption
Nitric acid plant consumption
Urea plant consumption
Electricity consumption [MW]
0
2
4
6
8
10
0
1000
2000
3000
4000
5000
6000
7000
Time [h]
Ammonia production
Nitric acid production
Urea production
CO2 emission
Production [tonnes]
0
50
100
150
200
250
300
0
1000
2000
3000
4000
5000
6000
7000
Time [h]
Ammonia storage [tonnes]
31000
31250
31500
31750
32000
32250
32500
32750
33000
Ammonia storage
0
1000
2000
3000
4000
5000
6000
7000

1.2 Simulation output BAU Scenario with High cost distribution

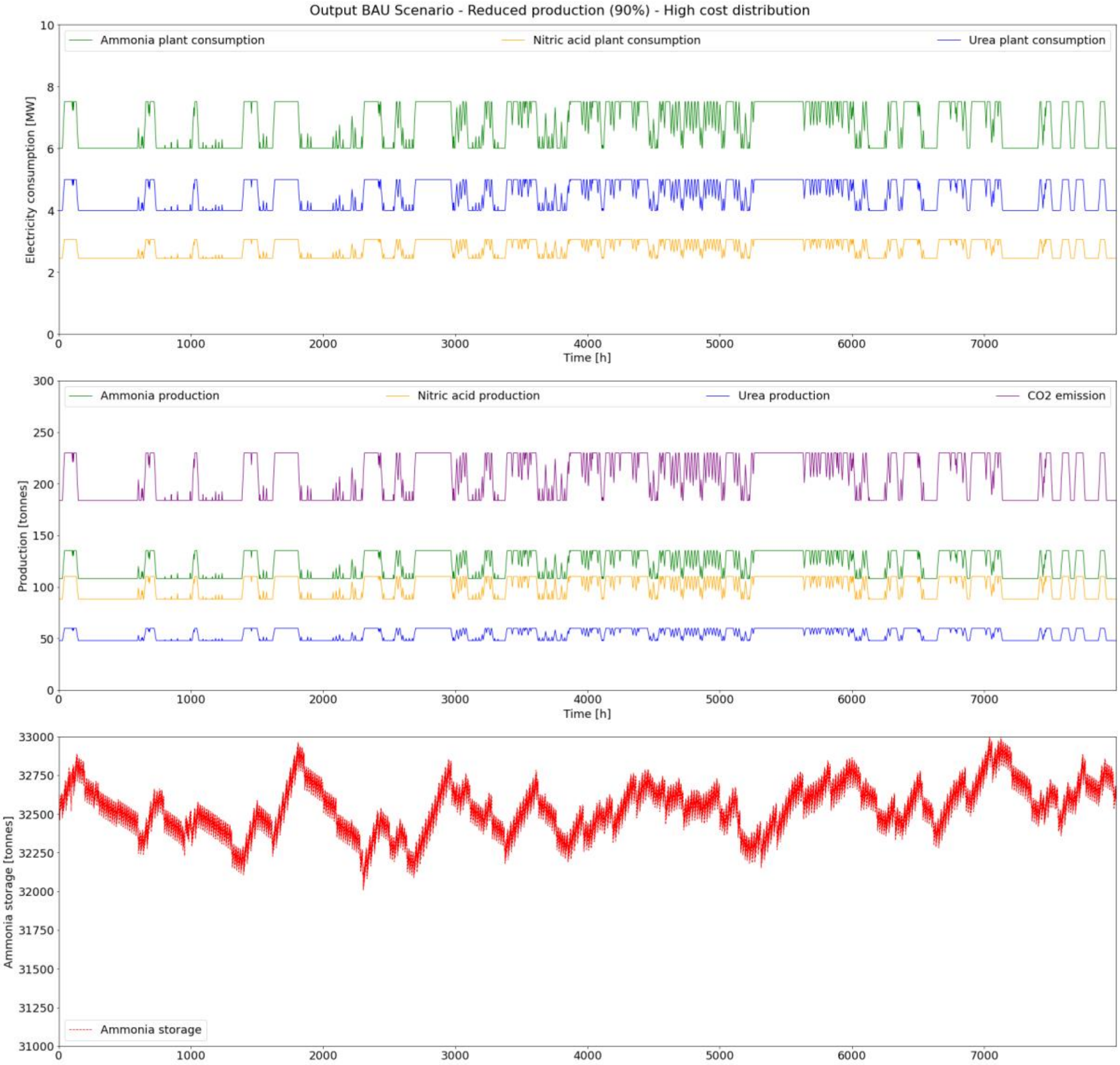
S1.A.ii



S1.B.ii


Output BAU Scenario - Increased load hours (8760) - High cost distribution
Ammonia plant consumption
Nitric acid plant consumption
Urea plant consumption
Electricity consumption [MW]
0
2
4
6
8
10
0
1000
2000
3000
4000
5000
6000
7000
8000
Time [h]
Ammonia production
Nitric acid production
Urea production
CO2 emission
Production [tonnes]
0
50
100
150
200
250
300
0
1000
2000
3000
4000
5000
6000
7000
8000
Time [h]
Ammonia storage
Ammonia storage [tonnes]
31000
31250
31500
31750
32000
32250
32500
32750
33000
0
1000
2000
3000
4000
5000
6000
7000
8000

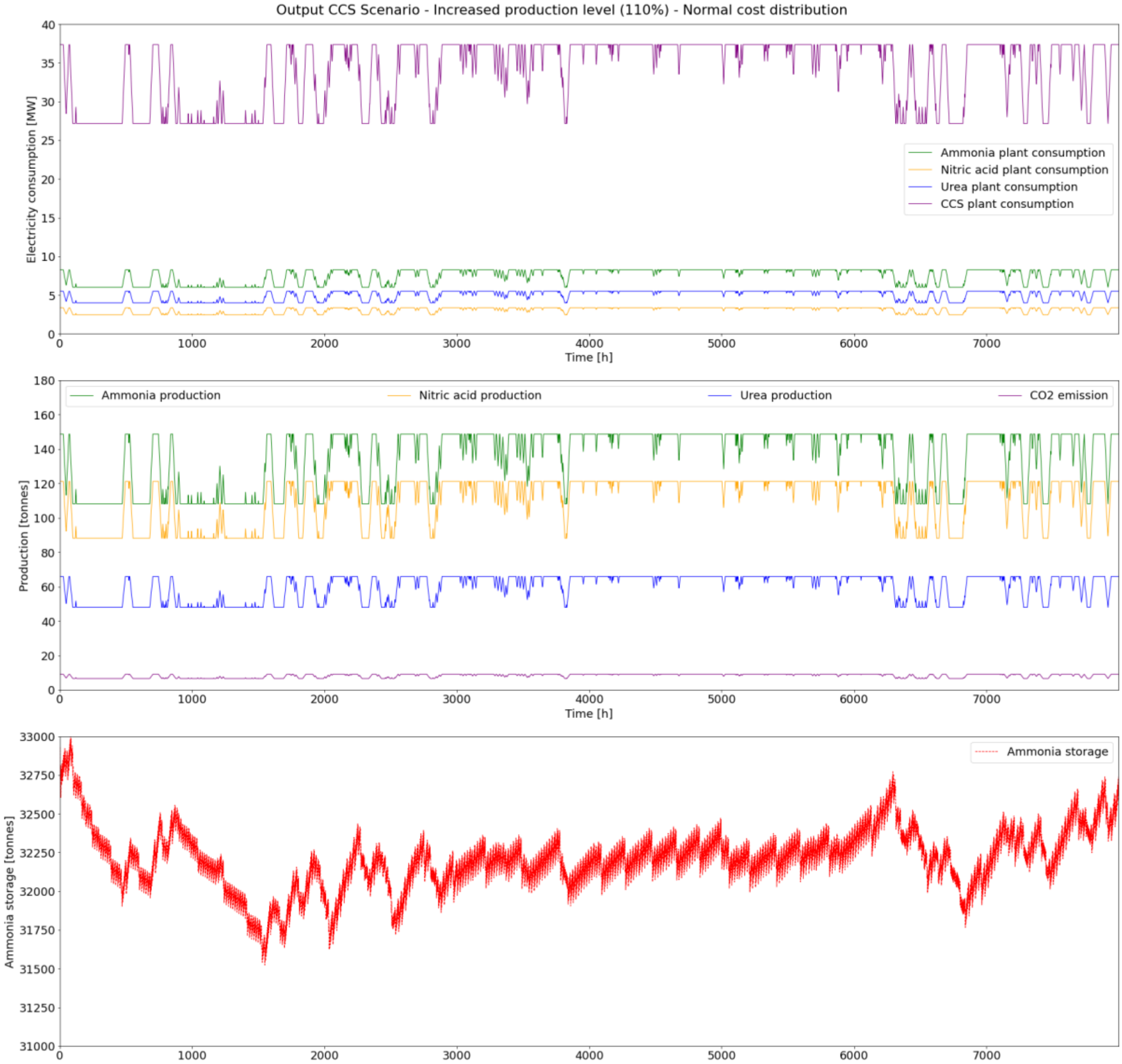
S1.C.ii


Output BAU Scenario - Reduced production (90%) - High cost distribution
Ammonia plant consumption
Nitric acid plant consumption
Urea plant consumption
Electricity consumption [MW]
0
2
4
6
8
10
0
1000
2000
3000
4000
5000
6000
7000
Time [h]
Ammonia production
Nitric acid production
Urea production
CO2 emission
Production [tonnes]
0
50
100
150
200
250
300
0
1000
2000
3000
4000
5000
6000
7000
Time [h]
Ammonia storage [tonnes]
31000
31250
31500
31750
32000
32250
32500
32750
33000
Ammonia storage
0
1000
2000
3000
4000
5000
6000
7000

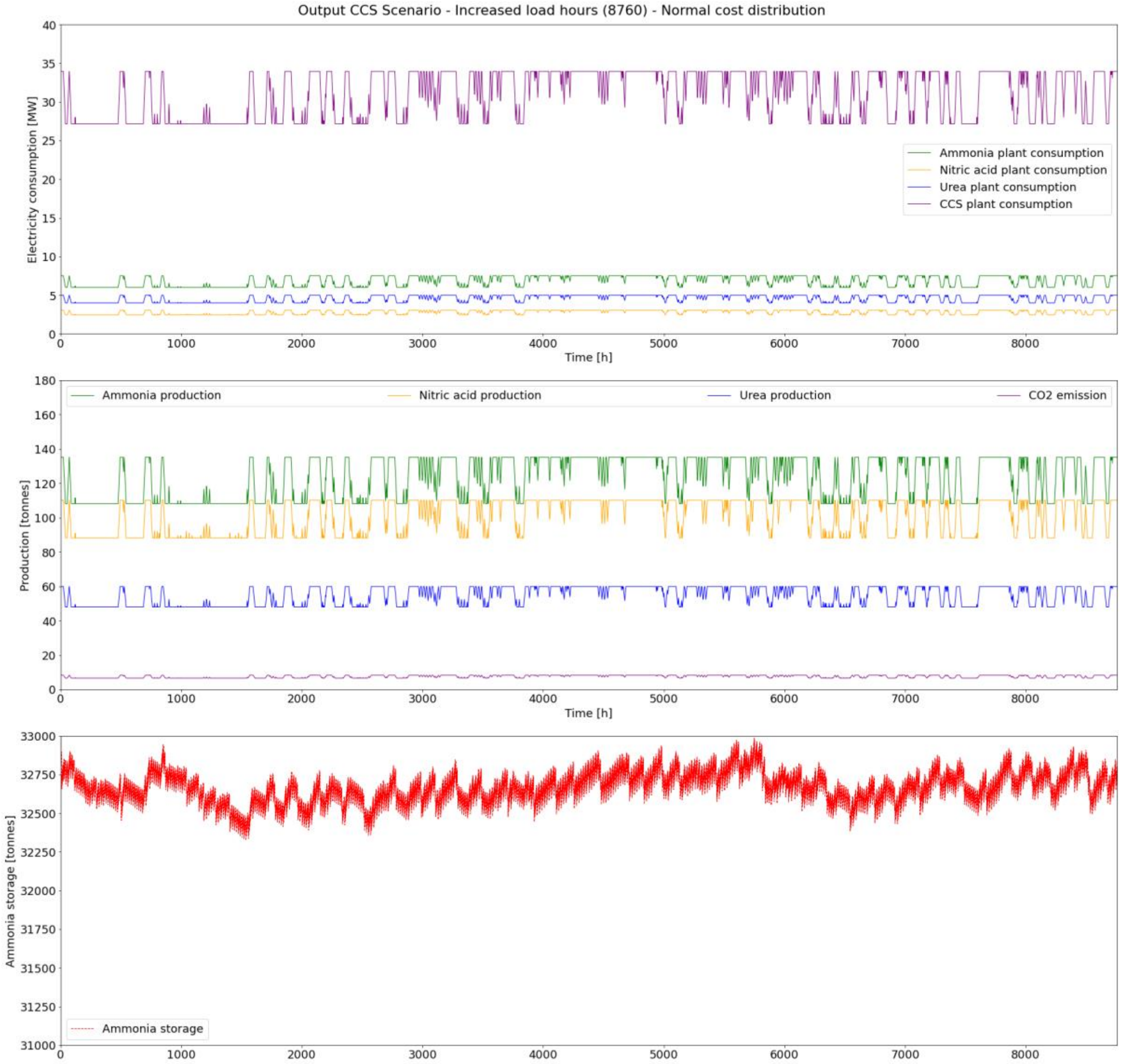
12.2 Appendix 2 CCS simulations

2.1 Simulation output CCS Scenario with Normal cost distribution

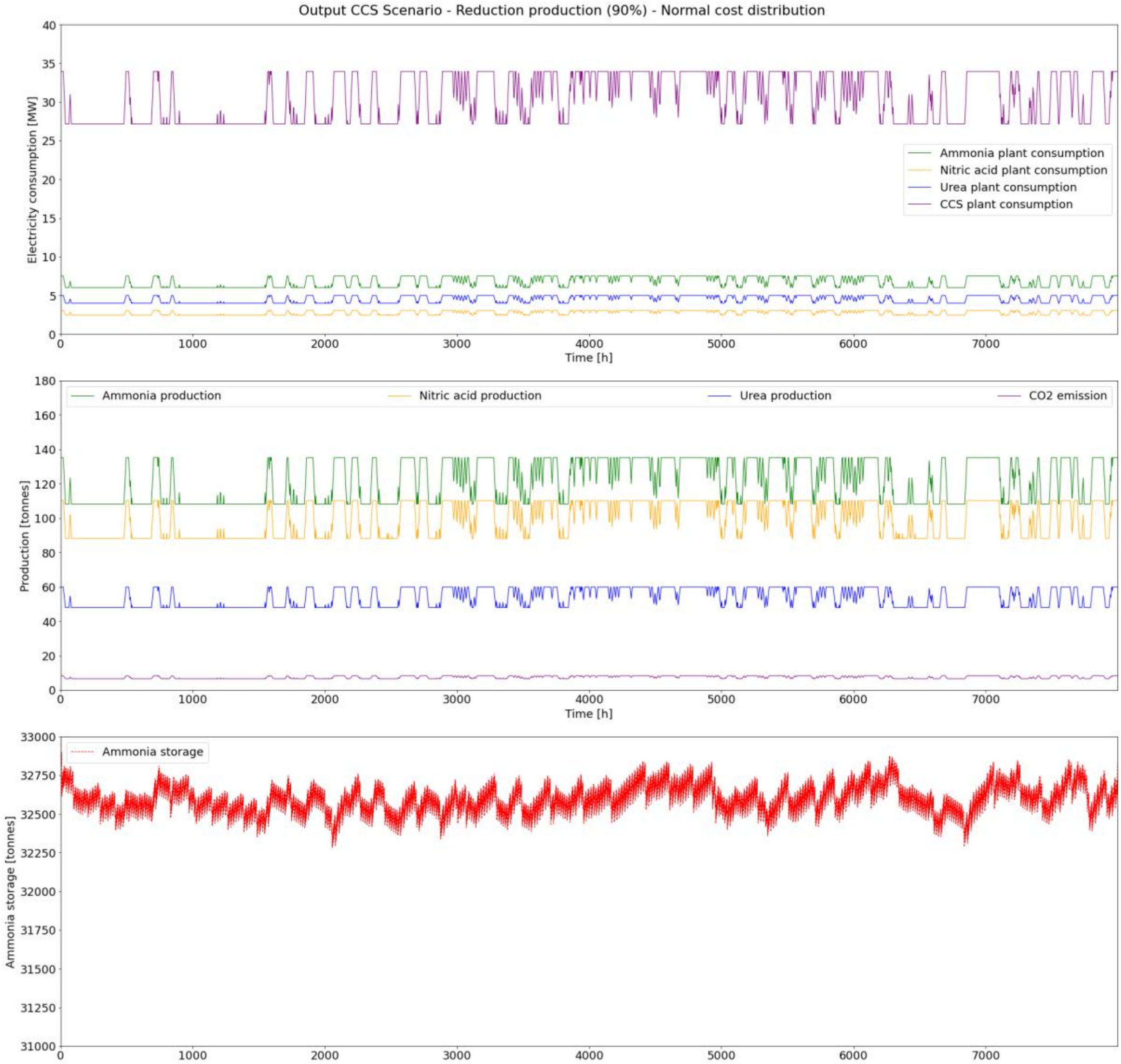
S2.A.i



S2.B.i

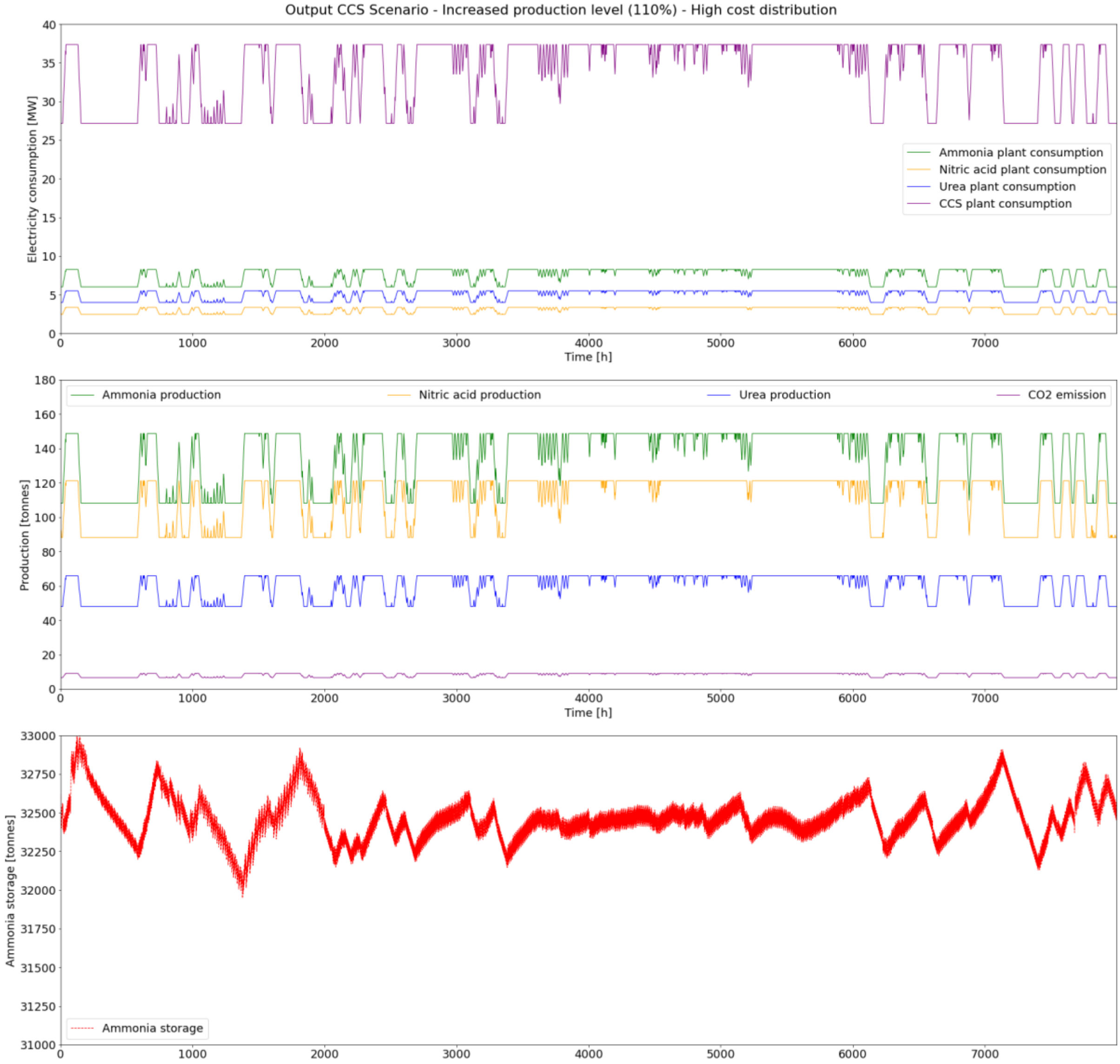

Output CCS Scenario - Increased load hours (8760) - Normal cost distribution
Electricity consumption [MW]
0
5
10
15
20
25
30
35
40
Ammonia plant consumption
Nitric acid plant consumption
Urea plant consumption
CCS plant consumption
Time [h]
0
1000
2000
3000
4000
5000
6000
7000
8000
Production [tonnes]
0
20
40
60
80
100
120
140
160
180
Ammonia production
Nitric acid production
Urea production
CO2 emission
Time [h]
Ammonia storage [tonnes]
31000
31250
31500
31750
32000
32250
32500
32750
33000
Ammonia storage

S2.C.i

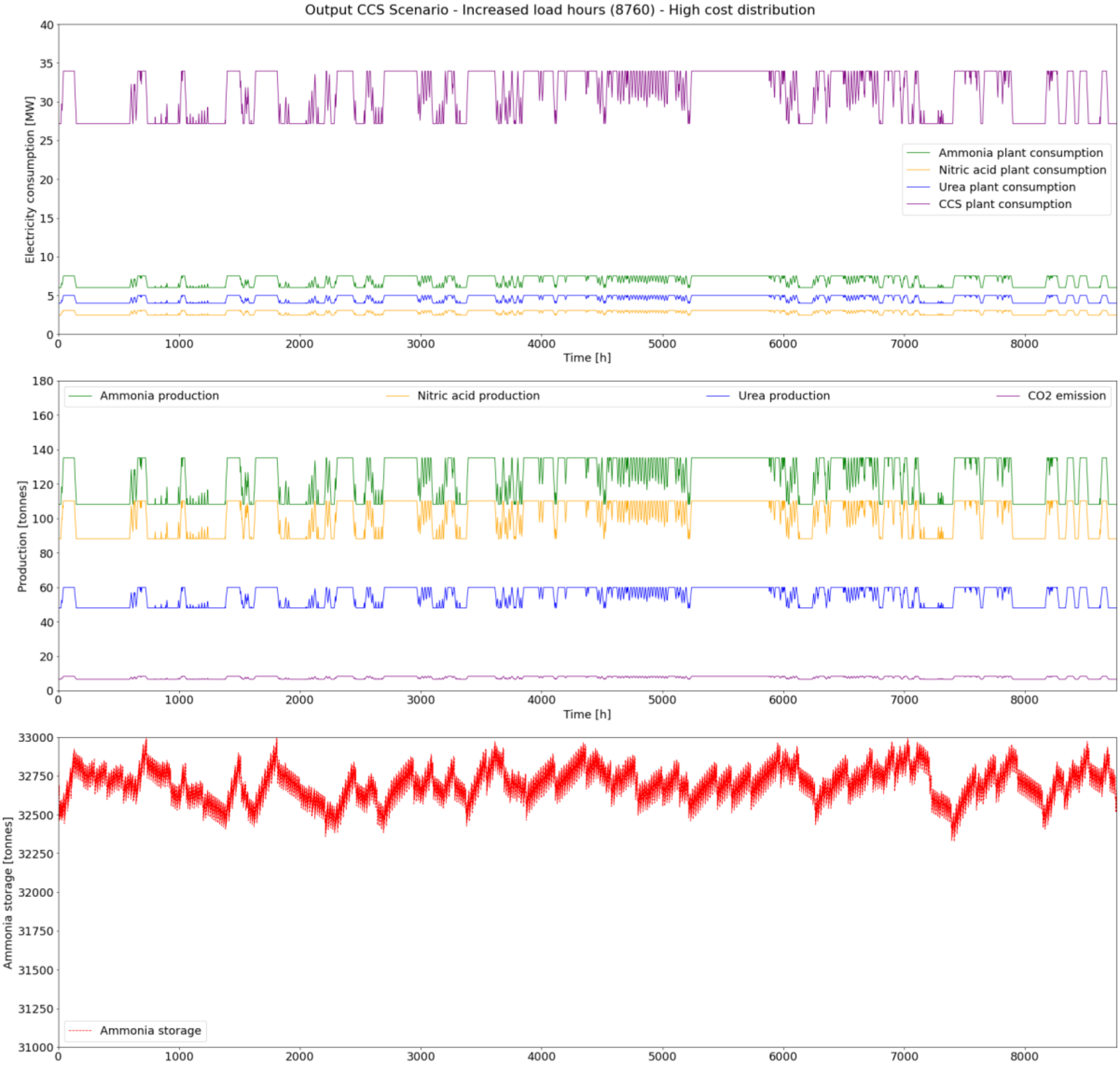

Output CCS Scenario - Reduction production (90%) - Normal cost distribution
Electricity consumption [MW]
40
35
30
25
20
15
10
5
0
Ammonia plant consumption
Nitric acid plant consumption
Urea plant consumption
CCS plant consumption
Time [h]
0
1000
2000
3000
4000
5000
6000
7000
Production [tonnes]
180
160
140
120
100
80
60
40
20
0
Ammonia production
Nitric acid production
Urea production
CO2 emission
Time [h]
Ammonia storage [tonnes]
33000
32750
32500
32250
32000
31750
31500
31250
31000
Ammonia storage

2.2 Simulation output CCS Scenario with High cost distribution

S2.A.ii



S2.B.ii


Output CCS Scenario - Increased load hours (8760) - High cost distribution
Electricity consumption [MW]
Ammonia plant consumption
Nitric acid plant consumption
Urea plant consumption
CCS plant consumption
Time [h]
Production [tonnes]
Ammonia production
Nitric acid production
Urea production
CO2 emission
Time [h]
Ammonia storage [tonnes]
Ammonia storage
0
1000
2000
3000
4000
5000
6000
7000
8000

S2.C.ii


Output CCS Scenario - Reduction production (90%) - High cost distribution
Electricity consumption [MW]
0
5
10
15
20
25
30
35
40
Ammonia plant consumption
Nitric acid plant consumption
Urea plant consumption
CCS plant consumption
Time [h]
0
1000
2000
3000
4000
5000
6000
7000
Production [tonnes]
0
20
40
60
80
100
120
140
160
180
Ammonia production
Nitric acid production
Urea production
CO2 emission
Time [h]
0
1000
2000
3000
4000
5000
6000
7000
Ammonia storage [tonnes]
31000
31250
31500
31750
32000
32250
32500
32750
33000
Ammonia storage
0
1000
2000
3000
4000
5000
6000
7000

12.3 Appendix 3 Green ammonia simulations

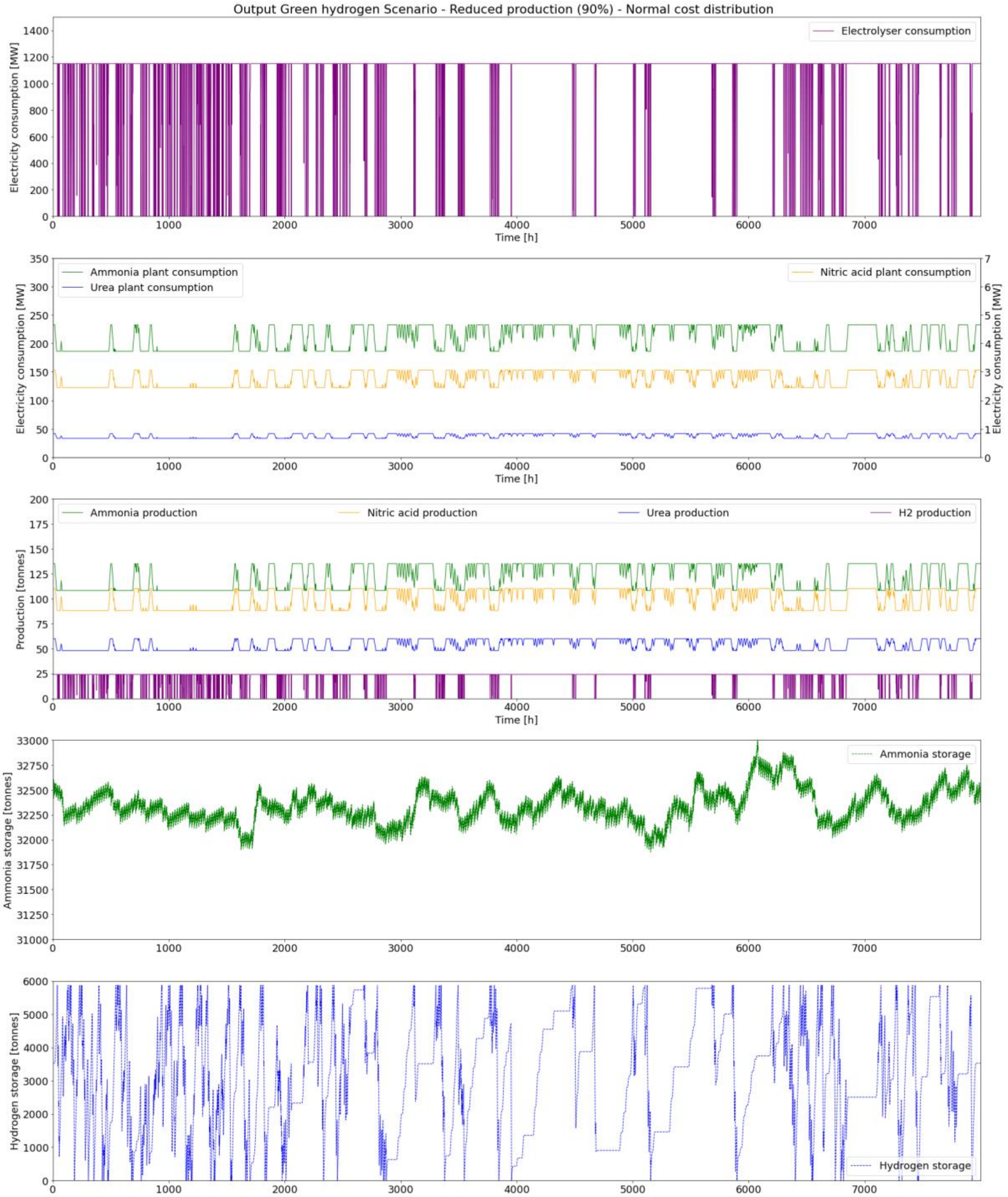
3.1 Simulation output Green Ammonia Scenario with Normal cost distribution

S3.A.i

S3.B.i


Output Green hydrogen Scenario - Increased load hours (8760) - Normal cost distribution
Electrolyser consumption
Electricity consumption [MW]
0
200
400
600
800
1000
1200
1400
Time [h]
0
1000
2000
3000
4000
5000
6000
7000
8000
Ammonia plant consumption
Urea plant consumption
Nitric acid plant consumption
Electricity consumption [MW]
0
50
100
150
200
250
300
350
1
2
3
4
5
6
7
Electricity consumption [MW]
Time [h]
Ammonia production
Nitric acid production
Urea production
H2 production
Production [tonnes]
0
25
50
75
100
125
150
175
200
Time [h]
Ammonia storage [tonnes]
31000
31250
31500
31750
32000
32250
32500
32750
33000
Ammonia storage
Hydrogen storage [tonnes]
0
1000
2000
3000
4000
5000
6000
Hydrogen storage

S3.C.i


Output Green hydrogen Scenario - Reduced production (90%) - Normal cost distribution
Electrolyser consumption
Electricity consumption [MW]
0
200
400
600
800
1000
1200
1400
Time [h]
0
1000
2000
3000
4000
5000
6000
7000
Ammonia plant consumption
Urea plant consumption
Nitric acid plant consumption
Electricity consumption [MW]
0
50
100
150
200
250
300
350
Electricity consumption [MW]
0
1
2
3
4
5
6
7
Time [h]
Ammonia production
Nitric acid production
Urea production
H2 production
Production [tonnes]
0
25
50
75
100
125
150
175
200
Time [h]
Ammonia storage
Ammonia storage [tonnes]
31000
31250
31500
31750
32000
32250
32500
32750
33000
Hydrogen storage
Hydrogen storage [tonnes]
0
1000
2000
3000
4000
5000
6000

3.2 Simulation output Green Ammonia Scenario with High cost distribution

S3.A.ii

S3.B.ii

Output Green hydrogen Scenario - Increased load hours (8760) - High cost distribution

S3.C.ii


Output Green hydrogen Scenario - Reduced production (90%) - High cost distribution
Electrolyser consumption
Electricity consumption [MW]
1400
1200
1000
800
600
400
200
0
1000
2000
3000
4000
5000
6000
7000
Time [h]
Ammonia plant consumption
Urea plant consumption
Nitric acid plant consumption
Electricity consumption [MW]
350
300
250
150
100
50
7
6
5
4
3
2
1
Ammonia production
Nitric acid production
Urea production
H2 production
Production [tonnes]
175
125
75
25
Ammonia storage
Ammonia storage [tonnes]
33000
32750
32500
32250
32000
31750
31500
31250
31000
Hydrogen storage
Hydrogen storage [tonnes]
6000
5000
4000
3000
2000
1000