TKP4170 PROCESS DESIGN PROJECT

Title: Energy efficient ammonia production plants	**Keyword (3-4):** Ammonia, Optimization, Aspen HYSYS
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Summary: Different types of feedstocks for production of ammonia were considered. The main focus was to find an energy efficient feedstock but also the magnitude of carbon emission was considered. After evaluating the different feedstocks, natural gas, electrolysis of water + nitrogen enriched air and coal, natural gas was considered to be the best option. Further, by investigating the compounds in natural gas, pure methane was evaluated to be the best feedstock due to the high hydrogen-carbon ratio.

After concluding on the feedstock, a HYSYS model of an ammonia plant, based on NII at Herøya, was made. The model was used to find any improvement on the operating conditions of the plant. The parameters that were evaluated were the front-end pressure, mole fraction in the air-inlet either by electrolysis of water or membrane separation of air, the steam-carbon ratio and the hydrogen-nitrogen ratio into the synthesis loop. These parameters were economically optimized by changing them independently whilst the other parameters were kept at their standard values. By doing so the optimal values for the parameters were found to be: p = 50 bar, $x_{O2,el}$ = 0.231, $x_{O2,mem}$ = 0.235, steam/carbon = 4.6 and H_2/N_2 = 2.6.

An investment and cost estimation of the different cases at their most profitable conditions were done. Further the internal rent of return, IRR, was calculated for all of the cases. By comparing the IRR for each of the cases to the standard case the conclusion for this study was made. Both the steam-carbon and the membrane case gave a higher IRR than the standard case. This implies that such suggested modifications can improve the profitability of an ammonia plant.

Conclusions and recommendations:

This study indicates that two of the cases were more profitability than the standard case. These were the steam-carbon and the membrane case. This conclusion comes from the fact that the IRR = 19.21% and 19.57% respectively. In comparison to IRR of 18.92%, for the standard case, this implies that the modifications in these cases would improve the profit of the plant. The high IRR for the steam carbon case is mainly due to a high gross profit, while for the membrane it is the low extra expenses compared to the extra ammonia produced.

A suggestion for further investigation is to combine different cases with the objective of finding an absolute optimum. It may also be suggested to investigate the affect of changing the inert concentration. Before doing so it will be beneficial to include kinetics, especially in the synthesis reactor, to improve the model. The most interesting result from this study was the increased production with an increased oxygen mole fraction in the air-inlet. Because of this a proposal would be to further investigate this.

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Contents

1 New technologies

1.1 Introduction

Ammonia production is one of the most important chemical processes in the modern world. The main use of ammonia is to produce nitrates which is further used to produce fertilizer. The most common way to synthesize the chemical is through the Haber Bosch synthesis where an approximate 3:1 mixture of hydrogen and nitrogen is pressurized to 100-300 bar and preheated before the reaction takes place over a catalyst, traditionally rich in iron, but different compositions is also used.

$$N_2 + 3\,H_2 \rightleftharpoons 2\,NH_3 \tag{1.1}$$

The product is separated at a low temperature before the unreacted material is recycled. However, the greatest variation between the different production plants is how the hydrogen is produced. The hydrogen production today is based on fossil fuels where light hydrocarbons are mainly used. China and India stands for the main usage of heavy hydrocarbons and coal. The carbon is oxidized by water to produce hydrogen and carbon monoxide, which is further oxidized in the water gas shift reaction. It is easily seen from the stoichiometry that methane is favorable due to high hydrogen-carbon ratio. Carbon dioxide is further removed from the process e.g. with absorption. The amount of carbon dioxide produced is proportional to the length of hydrocarbons in the feedstock. An alternative hydrogen production is through electrolysis of water which will eliminate the carbon emission given that the energy deficit comes from a renewable energy source.

In this section different feedstocks and corresponding processes for ammonia production was evaluated based on price, availability and carbon emissions.

1.2 Feedstocks

The energy requirement for different feedstocks using the best available technology is presented in table 1.1. Even though the energy consumption per ton ammonia, varies a lot all of the presented feedstocks are being used today. The feedstock used is dependent on availability, culture, technology and geography.

Table 1.1: Energy consumption and carbon dioxide emissions for diffrent feedstock types by using the best available technology per 2009 [1]

Energy source	Process	Energy GJ/ton NH_3	CO_2 emissions t/ton NH_3
Natural Gas	Steam reforming	28	1.6
Water	Electrolysis	34	0
Naphta	Steam reforming	35	2.5
Heavy Fuel Oil	Partial oxidation	38	3.0
Coal	Partial oxidation	42	3.8

1.3 Natural gas

Natural gas is the feedstock with the highest hydrogen-carbon ratio which implies lower carbon dioxide emissions and less energy demanding reactions. Using pure methane, half of the hydrogen production comes from the feedstock, and the other half from water. One of the main advantages of designing a plant based on natural gas is that the process is not very sensitive to variations in the feedstock composition.

In the production of ammonia, the gas is normally desulfurized because of the toxic behavior of sulfur on the catalyst. Further the gas is mixed with steam before the reforming reactions,(1.2),(1.3), takes place in a reformer.

$$C_nH_{2+2n} + nH_2O \rightleftharpoons nCO + (2n+1)H_2 \tag{1.2}$$
$$CO + H_2O \rightleftharpoons H_2 + CO_2 \tag{1.3}$$
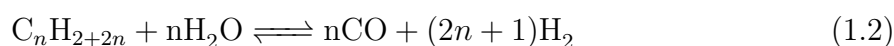
The outlet components are mainly hydrogen, carbon monoxide, carbon dioxide, methane and water. Air is then added in a secondary reformer where oxygen mainly reacts with methane, producing hydrogen and carbon monoxide (1.4),(1.5),(1.6).

$$2\,H_2O \rightleftharpoons O_2 + 2\,H_2 \tag{1.4}$$
$$2\,CH_4 + 3\,O_2 \rightleftharpoons 4\,H_2O + 2\,CO \tag{1.5}$$
$$CH_4 + 2\,O_2 \rightleftharpoons 2\,H_2O + CO_2 \tag{1.6}$$
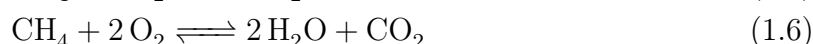
At this stage both nitrogen and hydrogen are present in the mixture, but the carbon oxides and water needs to be removed to prevent oxidation of the iron catalyst in the Haber Bosch synthesis. Water from the mixture can easily be removed by condensation and the carbon monoxide is removed by converting carbon monoxide to carbon dioxide by the water-gas shift reaction,(1.3), before the carbon dioxide is absorbed in water. The water can be added amines to improve the absorption. To prevent the remaining carbon oxides to enter the synthesis, two methanation reactions,(1.2 with n=1),(1.3), takes place before the gas is compressed. This reaction consumes hydrogen and is not

economically favorable, but is considered necessary. The gas is then compressed to 100-300 bar depending on the catalyst in the ammonia reactors. After being compressed, the gas is preheated before entering the reactors where the ammonia reaction,(1.2), occurs.

The gas is then cooled down before ammonia is separated by condensation. The remaining unreacted gas is then recompressed and fed to the reactors once again. This is called the synthesis loop. The amount of feedstock required, when natural gas is assumed to be pure methane, is 353.18 kg(CH_4)/ton(NH_3). The price of natural gas was 23.64 NOK/MMBtu in July 2016[2]. The different feedstock prices are summed up in table 1.2

To compare different light hydrocarbons a simulation model has been created using Aspen HYSYS V9. Reactors has been simulated using predetermined reaction sets which then goes to the thermodynamic equilibrium. For some of the reactor the outlet temperature is fixed. This simplification is done due to the lack of kinetic data for the different reactions with the different catalysts. The main usage for this model is to compare different feedstocks, so the approximations will be the same for the different simulation sets.

1.4   Electrolysis

An alternative method of producing hydrogen is by the use of alkaline electrolysers. Today there are no ammonia production plants using this method mainly because of economic reasons. However, using electrolysers, it is possible to produce ammonia without any carbon emissions if a renewable energy source is being used. The two renewable energy sources that are the most relevant is hydropower and solar cells, depending on the plant location. Another interesting aspect of this process is that the main feedstocks will be water and air, both very economically favorable feedstocks.

Alkaline electrolysis is a commonly used method for industrial use. A mixture of water and a soluble salt works as an electrolyte where its function is to transport electrons and ions. The container with electrolyte is connected to an external power source through electrodes in order for the electrons to travel through an external circuit and ions between electrodes[3].

One possible electrolyzer supplier is NEL, a company providing some of the best electrolysis technology today[4]. The hydrogen production using the NEL electrolyzers occur at temperatures between 70-90 $°C$ and 1-30 bar pressure. The cathode, which is where the hydrogen bubbles out, is made of nickel and steel whereas the anode, which is where the oxygen bubbles out, is made of nickel. The electrolyte contains 25-35wt% potassium hydroxide.

In the HYSYS model for natural gas as feedstock, the base was set to 1000 t/day ammonia. In order to produce 1000 t/day ammonia, or 41.7 t/h, an amount of 84404.7 Nm^3/h hydrogen is necessary. If NEL is used as the electrolyser supplier, an amount of 174 electrolysers, each with a maximum hydrogen production of 485 Nm^3/h , is required [5]. Each electrolyser requires 3.8 kWh/Nm^3 of hydrogen which means a total energy requirement for the desired hydrogen production is 320.737 MWh. The two renewable

energy sources considered is hydropower and solar cells. The total amount of hydropower produced in Norway is 30960 MW , which would mean that the use of this energy source would amount to 1.04 % of the total hydropower production in Norway [6]. Phenix power plant in Italy (REC) produces a maximum of 24 MW from 100 000 solar cell panels [7]. In order to fulfill the energy requirements of the hydrogen production from this kind of solar cell technology it would require 7.59 million solar cell panels, or 75.9 times the capacity of the italian-based power plant.

The amount of feedstock when hydrogen is produced by electrolysis, is $7.69 \, \mathrm{MWh/ton(NH_3)}$. The price of electricity is $2360.83 \, \mathrm{NOK/ton(NH_3)}$[8].

1.5   Nitrogen enriched air

If the hydrogen is produced from electrolysis, the oxygen is no longer required. In this case nitrogen enriched air could become relevant. To produce 95% nitrogen at 9 barg on the basis of $15000 \mathrm{Nm^3/h}$ the energy requirement is approximately $870 \mathrm{kJ/Nm^3}$. The energy consumption comes from compressors when membrane separation is used. Alternatives to membrane separation are cryogenic separation of air and pressure swing adsorption (PSA), but this is more energy demanding (Haugland, Christer, Air Products, 07.09.16, Appendix C).

1.6   Coal

Gasification of coal has been used for several years in producing syngas, which is further used in production of ammonia. Due to the high prices of oil and natural gas, the gasification process has been preferred in many countries. China has been the largest producer of ammonia from coal over the past 15 years, and in 2006 they had 75 % of the production [9].

The main disadvantage of coal gasification is the energy consumption. The first ammonia plant had an energy use of about 45 GJ/t NH3, which is a much higher energy consumption than the other processes mentioned.

The chemical reactions in the gasification process,(1.3),(1.7), can progress to different extents depending on the gasification conditions, temperature and pressure. The gasification proceeds as follows to produce syngas[10]:

$$3 \, \mathrm{C} + \mathrm{O_2} + \mathrm{H_2O} \rightleftharpoons 3 \, \mathrm{CO} + \mathrm{H_2} \qquad (1.7)$$

Hydrogen is the desired end-product, so the carbon monoxide undergoes the water gas shift reaction(1.3).

The coal gasification process can be classified according to method. There are three gasification methods mainly used; Lurgi process, Winkler process and Koppers-Totzek

process. The Lurgi process is characterized by adding coal at the top of the gasifier which descends countercurrently to the gas stream. This countercurrent method results in high thermal efficiency and good heat exchange, and therefore it requires less heat and oxygen than the other processes. Also oxygen with a purity of less than 90% is used. The product gas from the Lurgi process has a temprature of 450°C and contains 16.9% carbon monoxide, 39.4% hydrogen, 9% methane and 31.5% carbon dioxide. Characteristics for the Winkler process is that the steam and the oxygen are injected near the bottom of a fluidized bed. The fluidized bed is isothermal with a temprature of 1000 ^{o}C, so the exit gas mainly contains hydrogen and carbon monoxide with less than 1% methane. A disadvantage of this process is high compression cost (1-3 atm). Koppers-Totzek process is the most used coal based ammonia plant nowadays. The fine graded, dried coal is picked up by a stream of oxygen and blown into a gasification chamber through two burners facing each other. The exit gas in Koppers-Totzek process is 52.5% carbon monoxide, 36% hydrogen and 10% carbon dioxide. The need of fine graded coal and operation at low pressures (1-3 atm) is the main disadvantages of this process. The high amount of carbon monoxide and carbon dioxide in the exit gas as well as the high compression costs, is the main drawbacks with these methods of producing ammonia [11], [12].

The reguired feedstock of coal is 528.89 kg (C)/ton NH_3 (assuming coal only contains carbon). The price of coal (South African coal) in July 2016 was 533.78 NOK/ton [2]. The calculated cost of coal as feedstock is 282.32 NOK/ton NH_3. This results in a lower feedstock price for coal than for natural gas as shown in 1.2. The heating value for carbon is -17.35 GJ/ton NH_3, which compared to the value for natural gas, is a bit lower.

1.7 Economics

Table 1.2 shows the amount of feedstock needed to produce one ton of NH_3 and the related heating value. The values are further used in calculating the prices in table 1.3.

Table 1.2: Amount of feedstock and heating value for different types of feedstock.

Feedstock	Amount of feedstock	HHV GJ/ton NH_3	Feedstock price NOK/ton NH_3
Natural Gas	353.18 kg/ton NH_3	-17.7	414.87
Electrolysis	7.69 MWh/ton NH_3		2360.83
Nitrogen enriched air	0.160 MWh/ton NH_3		49.12
Coal	528.89 kg/ton NH_3	-17.35	282.31

Table 1.3: Calculated prices and profits for different feedstocks. The profit in this table is the difference between the cost of feedstock and the income from selling the ammonia with a ammonia price of 2321 NOK/ton[13].

Feedstock	Price	Feedstock price NOK/ton NH_3	Profit NOK/ton NH_3
Natural Gas	1.175 NOK/kg [14]	414.87	1906.27
Electrolysis + NEA	0.307 NOK/kWh[8]	2409.95	-88.55
Coal	0.534 NOK/kg[2]	282.31	2038.83

1.8 Conclusion - Further investigating

Based on energy consumption it is clearly an advantage using methane which also has the lowest carbon emissions among the fossil feedstocks. It is also interesting to investigate the electrolysis process because of this being the green alternative, but the huge requirement for electric power makes hydrogen from electrolysis non beneficial. The coal and heavier hydrocarbon feedstocks will be discarded from further investigation due to high energy requirements and carbon emissions.

The HYSYS model which is based on a methane as feedstock has shown an increase in the hydrogen production when oxygen levels in the air are increased about 2 %. The extra oxygen can be derived from electrolysis where the extra hydrogen can be fed into the process after the absorption towers.

Further investigations will be performed using the HYSYS model. The focus will be to optimize the profit with respect to different variables which will be investigated independently.

2 Design Basis

This model is based on the ammonia factory, NII, on Herøya, Porsgrunn. ASPEN HYSYS V9 was used for the simulations.

- The feedstock was 20 ton/h of pure methane.

- The sulfur removal was neglected as the feedstock was assumed to be pure methane.

- The filtering and de-ionization process of water used for steam production was neglected.

- The air is assumed to contain 78% nitrogen, 21% oxygen and 1% argon.

- All reactors was modeled as Gibbs reactors. That is, it was assumed that the reactor outlets are at thermodynamic equilibrium.

- The reactions in the steam reformer and secondary reformer was assumed to be all the linearly independent reactions found from the null space of the atom-species matrix of the current reactants and the products carbon monoxide, carbon dioxide and hydrogen.

- In the water-gas shift reactors it was assumed that the water-gas shift reaction is the only reaction that occurs, thereby neglecting the production of both ammonia and biproducts such as methanol.

- The reaction set in the methanation reactor was assumed to only contain the methanation of carbon monoxide and carbon dioxide.

- For the synthesis reactor it was assumed that the only reaction is the ammonia production from hydrogen and nitrogen. The outlet temperature was fixed to 300°C.

- The outlet temperature of the steam reformer was fixed to 731 °C by adjusting the energy stream into the reactor.

- The amount of additional CH_4 needed for combustion in the steam reformer was calculated from the energy stream attached to the steam reformer in addition to heating the combustion products up to 760°C.

- The residence time, τ, for R-2, R-3, R-4 and R-5 was assumed to be 5 seconds.

- The residence time, τ, for the synthesis reactor, R-6, was assumed to be 33 seconds.

- The inert concentration in the synthesis loop was assumed to be 10 mole-%

- The recycle of the purge was not included in the model, but it was assumed 100% recovery of the ammonia in the purge and that all of the hydrogen and methane was used as fuel in the steam reformer.

- The flash from depressurizing the ammonia stream was recompressed and led back to the synthesis loop.

- All compressors was assumed to be adiabatic with an efficiency of 75%.

- All heat exchangers was modeled as heaters and coolers.

- No heat integration was performed, but an exergy balance was done instead.

- All pressure drops over the units were modeled as pressure drops over valves.

- The absorption of carbon dioxide was done with pure water. The mole fraction of carbon dioxide out the absorption towers was set to be 0.3%.

- The process for removing carbon dioxide from the water was not included.

- The price for electricity was assumed to be constant and 0.3 NOK/kWh.

- The price for MP steam was assumed to be constant and 82.1 NOK/ton.

- The price for ammonia was assumed to be constant and 2321 NOK/ton.

- The factor between thermochemical energy to electrical energy was assumed to be 0.6.

- The void fraction, ϕ, for the reactors R-2 to R-6, was set to 0.45.

- The length of the tubes in the primary reformer was assumed to be 10 meters and consisting of nickel and inconel.

- The cost calculations for the primary reformer only include the cost of the pipes.

- The heaters and coolers were assumed to be U-tube shell and tube exchangers.

- The heat transfer coefficient, U, was set to 400 W/m^{2}K.

- The separators were assumed to contain demister pads

- The minimum hold up of liquids in separators were assumed to be 10 minutes

- The absorbers was assumed to consist of 15 stages, with 0.5 m in between. Including the top and bottom space the total height was assumed to be 9.5 m. In addition the diamater was set to be 1.5 m.

- The pumps were assumed to be single-stage centrifugal pumps. In addition it was assumed that the equation 5.15 could be used even though the sizing parameter exceeds the upper limit.

- It was assumed 352 production days per year

- Working capital was assumed to be 5% of C$_{FC}$.

- The cost of water and waste disposal was excluded.

- The temperature in and out of the combustion chamber was assumed to be 760 and 220°C

- The cost of methane was assumed to be the same as the cost of natural gas.

- The operator salaries were assumed to be 500 000 NOK per year.

- The direct salary overhead was assumed to be 40% of operating salaries plus supervision.

- Maintenance was calculated as 3% of ISBL.

- The property taxes and insurance was calculated as 1% of ISBL.

- Costs such as rent of land, general plant overhead, capital charges, sales and marketing cost were excluded.

- The flue gas was assumed to be heat exchanged after R-1 to calculate the energy available after the combustion in the primary reformer.

- The tax percentage was assumed to be 28%.

3   Process Description
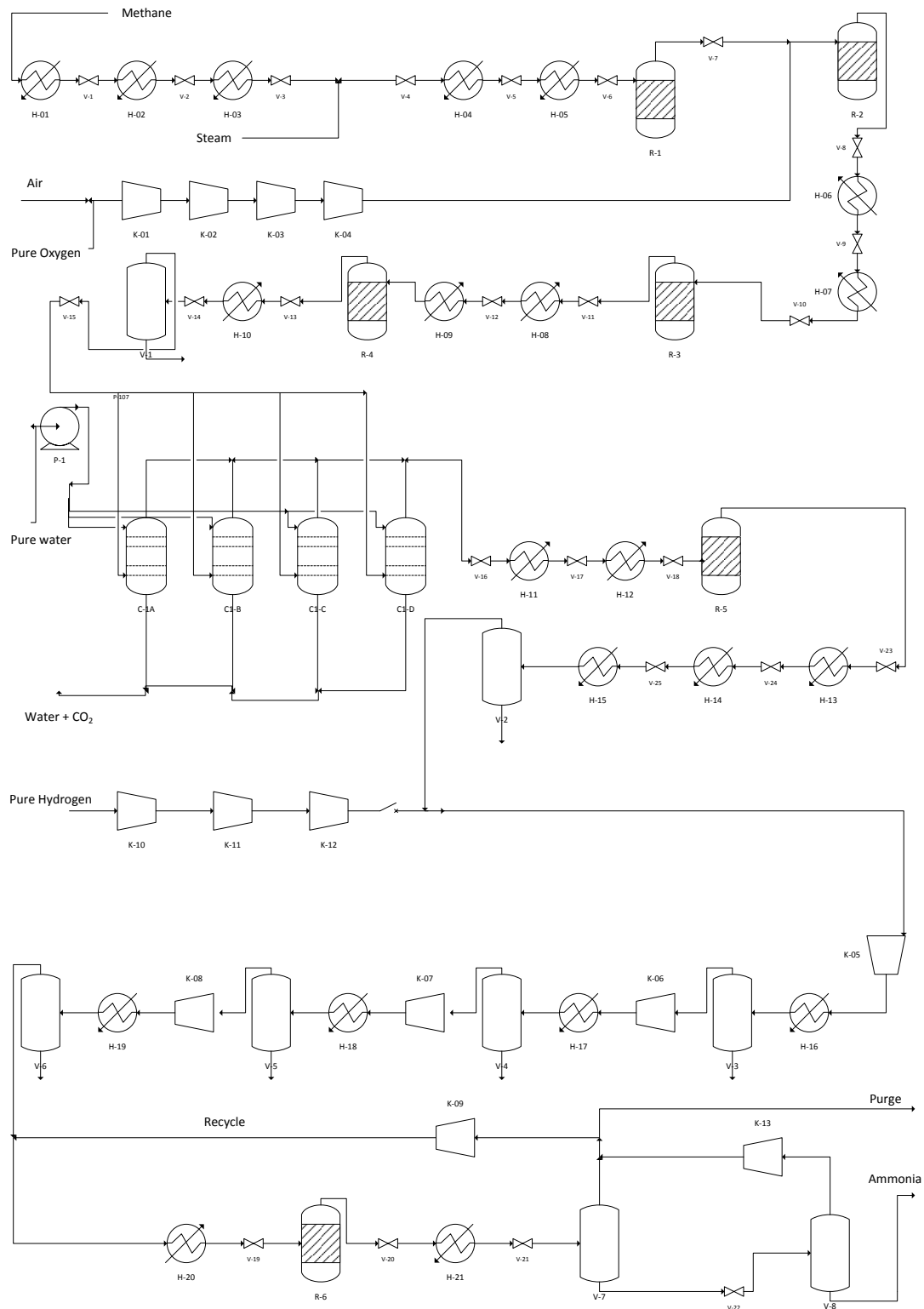
Figure 3.1: Process flow diagram, PFD, of the HYSYS model of the ammonia plant.

This process description is based on the standard case. This means using the conditions and values which best match the plant at Herøya using methane as a feedstock and using the assumptions and simplifications described in the design basis.

The feedstock in this model is pure methane which comes into the plant with a temperature of 14°C and 60 bar. The first step of the process is to preheat the methane. This is done over three heat exchangers where the pressure drop is simulated with valves in between the exchangers. This is the general case for the pressure drop simulations in this model. After the heat exchangers the methane has a pressure of 30 bar and a temperature of 150°C. The methane is then mixed with medium pressure steam. The steam to carbon ratio was set to 3.5. An excess of steam is added to prevent the formation of free carbon in the primary reformer. After the steam is mixed with the methane, the gas is further preheated in two heat exchangers before entering the primary reformer with a temperature of 520°C and a pressure of 27 bar. In the primary reformer methane reacts with water to form hydrogen, carbon monoxide and carbon dioxide described with the following reactions;

$$CH_4 + H_2O \rightleftharpoons 3\,H_2 + CO \tag{3.1}$$
$$CH_4 + 2\,H_2O \rightleftharpoons 4\,H_2 + CO_2 \tag{3.2}$$
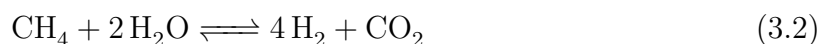
The design of the primary reformer is a large combustion chamber with vertical pipes going through. Since the reactions in the primary reformer is highly endothermic, large amounts of energy is needed here. The energy required is derived from hydrogen and methane coming from the ammonia synthesis purge in addition to extra methane being combusted on the outside of the pipes. The temperature out of the primary reformer was fixed at 730°C. The combustion products, often called flue gas, is cooled down to approximately 200°C before being released into the atmosphere.

Leaving the primary reformer the process gas is mixed with air. The amount of air added was fixed to get a hydrogen/nitrogen ratio of 3 into the synthesis gas compressor. The air, being the nitrogen source for the ammonia, is compressed from an atmospheric pressure and a temperature of 15°C up to the same pressure as the process gas. This is done over four compressor stages where the pressure ratio is evenly distributed over the stages. The adiabatic efficiency was set to 75%. Here the compression is purely adiabatic with no cooling. This gives the air which is leaving the compressor a temperature of approximately 635°C. The mixture then enters the secondary reformer where the following reactions occur;

$$2\,H_2O \rightleftharpoons O_2 + 2\,H_2 \tag{3.3}$$
$$2\,CH_4 + 3\,O_2 \rightleftharpoons 4\,H_2O + 2\,CO \tag{3.4}$$
$$CH_4 + 2\,O_2 \rightleftharpoons 2\,H_2O + CO_2 \tag{3.5}$$
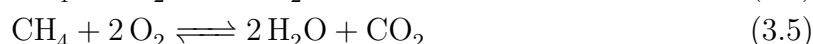
Leaving the secondary reformer the process gas contains hydrogen, nitrogen, argon, methane, water, carbon monoxide and carbon dioxide. The temperature out of the sec-

ondary reformer is 895°C with a pressure of 26.5 bar. The gas is then cooled down to 338°C with a pressure of 25.5 bar using two large heat exchangers. The gas then enters the first of two shift reactors where the water-gas shift reaction takes place;

$$H_2O + CO \Longrightarrow H_2 + CO_2 \tag{3.6}$$

The gas is cooled down from 403°C to 203°C before entering the second shift reactor. The process gas is then cooled to 36°C and water is removed using a separator. At this stage the carbon monoxide level is less than 1200 ppm. The next step is to remove the carbon dioxide. This is done by absorbing it in water using 4 absorbtion towers. The absorbant is pure water and not a water-amine mixture which is much more commonly used. The water used in the towers is pressurized to a pressure equal to that of the process gas using a pump on each of the absorbtion towers. The outlet concentration of carbon dioxide from the absorbtion towers was fixed at 0.3%. After leaving the absorption towers the process gas has a temperature of 6°C and a pressure of 23 bar. The gas is then preheated to 314°C before entering the methanation reactor. Here the remaining carbon monoxide and carbon dioxide is removed by the following reactions;

$$CH_4 + H_2O \Longrightarrow 3\,H_2 + CO \tag{3.7}$$
$$4\,H_2 + CO_2 \Longrightarrow CH_4 + 2\,H_2O \tag{3.8}$$
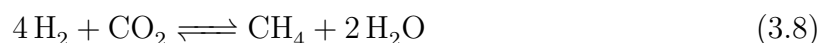
Methane and argon will act as inerts in the remaining parts of the process. The formation of methane from carbon oxides will use up some of the hydrogen, but this is necessary because oxides will poison the synthesis catalyst. After the methanation reactor the process gas is cooled to 14°C and water is removed using a separator. Entering the compressor the process gas contains hydrogen and nitrogen with a ratio of 3, in addition to water, methane and argon. The gas into the compressor has a pressure of 22 bar. The gas is then compressed up to 235 bar using 4 compressor stages with cooling and water separation between the stages. The pressure ratio is evenly distributed between the stages. Leaving the compressor the gas proceeds into the synthesis loop. Here it will mix with the synthesis gas already in the loop before it is preheated to 200°C. Then it comes into the ammonia reactor where the following reaction takes place;

$$N_2 + 3\,H_2 \Longrightarrow 2\,NH_3 \tag{3.9}$$

The reactor has a fixed outlet temperature of 300°C which is controlled using an internal cooler in the reactor. The gas leaving the ammonia reactor is then cooled to 5°C before it enters a separator which separates out the condensed ammonia. The liquid stream from this separator is depressurized to 5 bar using a valve. The temperature here is about -8°C. The liquid then enters a flash tank where impurities can flash off from the liquid ammonia. The flash gas is recompressed and put back into the synthesis loop. The liqiud

stream leaving the flash tank is the ammonia product. This has a purity of approximately 99.8%. The flash gas is mixed with the gas which leaves the ammonia separator and flows back to be mixed with the gas leaving the compressor. On this loop a purge stream is used to control the concentration of the inerts methane and argon. The sum of these mole fractions was kept at 10% using this purge. The total pressure drop in the loop was set to be 10 bar where the gas coming back to the outlet of the compressor is repressurized using an additional compressor.

3.1 Cases

After the standard model, also called the standard case had been established, multiple variables were investigated independently. These variables were the pressure of the methane coming into the factory, the steam to carbon ratio, the synthesis loop pressure, the hydrogen to nitrogen ratio coming into the synthesis compressor and the mole fraction of oxygen in the air entering the air compressor. The manipulation of the oxygen mole fraction was done by adding a stream of pure oxygen to the already existing air stream coming into the air compressor. The stream of oxygen can be produced either using electrolysis of water or using membrane separation of air.

3.1.1 Front-end pressure

Looking at the composition out of the secondary reformer, it can be seen that methane has a mole fraction of approximately 0.2%. This methane will go unconverted through the rest of the process acting as an inert. It will be beneficial to further reduce the content of methane out of the secondary reformer. Looking at the stoichiometry of the equations, 3.1-3.5, in the primary and secondary reformer it can be seen that the preference will be towards the product side when the pressure is lowered according to Le Chateliers principle. The main assumption here was that the gas leaving the primary and secondary reformer actually is in equilibrium, which is true for the model used in this experiment.

A result from lowering the pressure in the inlet methane is that the pressure is also lowered before the synthesis gas compressor. This will give additional shaft work requirements. Another effect is that a lower pressure will give a less effective absorbtion of carbon dioxide in water, since the outlet concentration of carbon dioxide was set to fixed value the amount of water needed to meet this requirement will increase. This will give an increase in the work done by the water pumps.

3.1.2 Hydrogen-nitrogen ratio

From an equilibrium point of view the ammonia reaction, 3.9, will prefer a lower ratio than 3 to produce ammonia. Lowering the ratio means increasing the amount of air coming into the process. This will increase the shaft work on both the air compressor and on the synthesis gas compressor because of the increased amount of gas.

3.1.3 Steam-carbon ratio

Stoichiometry from the chemical equations used in the primary reformer shows a preference towards the product side when the amount of water is increased. The same can be shown for the water-gas shift reaction, 3.6. This means increasing the amount of steam which is added to the process gas before the primary reformer. This will give an additional cost for the extra steam needed.

3.1.4 Mole fraction oxygen by membrane

Additional oxygen, being on the reactant side of the chemical equations related to the secondary reformer, will give an increase in hydrogen production. The extra oxygen in this case produced using membrane technology. The energy needed to operate a membrane separation unit is taken into account as well as the additional compressor work needed to compress the extra gas.

3.1.5 Mole fraction oxygen by electrolysis

An alternative to membrane separation of air is electrolysis of water. Here, the oxygen produced can be assumed to be pure and in addition twice the amount of hydrogen is produced. The extra hydrogen, also being pure, can be compressed and added to the main process gas entering the synthesis gas compressor in order produce more ammonia. The main disadvantage here is that electrolysis of water requires large amounts of electricity. Furthermore extra compressors will be needed to compress the additional hydrogen produced from the electrolysis. In addition electrolyzers are needed.

3.1.6 Synthesis loop pressure

Since the ammonia reaction,3.9, has a 4:2 ratio towards the product side it will be natural to expect an increase in the production when the pressure is increased from an equilibrium point of view. This will increase the compressor work done by the synthesis gas compressor.

4 Flowsheet calculations

All results presented in this section was calculated by the model of the ammonia plant modeled in Aspen HYSYS. The synthesis loop pressure case is excluded from further investigations as the results clear trend could not be found.

4.1   Standard Case

In the standard case the following input data was used: $p_{in} = 60$ bar, $x_{O_2} = 0.21$, Steam/Carbon = 3.5, $H_2/N_2 = 3$ and $p_{synthesis} = 235$ bar.

4.1.1   Stream conditions

The most important conditions in and out of the main units in the standard case is presented in table 4.1.

Table 4.1: Conditions in and out of the units in the ammonia plant model calculated by HYSYS with standard conditions. $p_{in} = 60$ bar, $x_{O_2} = 0.21$, Steam/Carbon = 3.5, H_2/N_2 = 3 and $p_{synthesis} = 235$ bar.

Stream	Vapor fraction [-]	Temperature [°C]	Pressure [bar]	Molar flow [kmol/h]
Inlet	1.0000	14	60.0	1247
Steam	1.0000	330	30.4	4363
R1 in	1.0000	521	27.2	5610
R1 out	1.0000	715	26.6	6943
Air	1.0000	15	1	1705
Comp. Air	1.0000	634	26.6	1705
Oxygen	-	-	-	-
R2 in	1.0000	730	26.6	8648
R2 out	1.0000	896	26.5	9339
R3 in	1.0000	338	25.6	9339
R3 out	1.0000	403	24.7	9339
R4 in	1.0000	203	24.2	9339
R4 out	1.0000	217	23.9	9339
V1 in	0.7117	36	23.8	9339
V1 top	1.0000	36	23.6	6646
C1 in	1.0000	36	23.6	6646
C1 out	1.0000	6	23.3	5452
R5 in	1.0000	314	22.6	5452
R5 out	1.0000	346	22.5	5398
V2 in	0.9923	14	22.2	5398
V2 top	1.0000	14	22.2	5356
Hydrogen	-	-	-	-
V3 in	0.9997	15	39.9	5356
V3 top	1.0000	15	39.9	5355
V4 in	0.9998	15	72.1	5355
V4 top	1.0000	15	72.1	5354
V5 in	0.9999	15	130.2	5354
V5 top	1.0000	15	130.2	5353
V6 in	~1.0000	15	235	5353
V6 top	1.0000	15	235	5353
R6 in	1.0000	200	235	7617
R6 out	1.0000	300	235	5085
V7 in	0.4427	5	225	5085
V7 top	1.0000	5	225	2251
V7 btm	0.0000	5	225	2834
V8 in	0.1200	-9	5	2834
V8 top	1.0000	-9	5	340
Ammonia	0.0000	-9	5	2494
Purge	1.0000	77	225	327
Recycle	1.0000	82	235	2264

4.1.2 Mole fractions

The mole fractions of the components in and out of the main units in the standard case is presented in table 4.2.

Table 4.2: Mole fractions in and out of the units in the ammonia plant model calculated by HYSYS with standard conditions. p_{in} = 60 bar, x_{O_2} = 0.21, Steam/Carbon = 3.5, H_2/N_2 = 3 and $p_{synthesis}$ = 235 bar.

Stream	x_{CH_4}	x_{H_2O}	x_{CO_2}	x_{CO}	x_{H_2}	x_{N_2}	x_{Ar}	x_{O_2}	x_{NH_3}
Inlet	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Steam	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
R1 in	0.2222	0.7778	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
R1 out	0.0836	0.4697	0.0627	0.0333	0.3507	0.0000	0.0000	0.0000	0.0000
Air	0.0000	0.0000	0.0000	0.0000	0.0000	0.7800	0.0100	0.2100	0.0000
Comp. Air	0.0000	0.0000	0.0000	0.0000	0.0000	0.7800	0.0100	0.2100	0.0000
Oxygen	-	-	-	-	-	-	-	-	-
R2 in	0.0671	0.3771	0.0504	0.0267	0.2816	0.1538	0.0020	0.0414	0.0000
R2 out	0.0060	0.3604	0.0559	0.0716	0.3618	0.1424	0.0018	0.0000	0.0000
R3 in	0.0060	0.3604	0.0559	0.0716	0.3618	0.1424	0.0018	0.0000	0.0000
R3 out	0.0060	0.3018	0.1145	0.0130	0.4204	0.1424	0.0018	0.0000	0.0000
R4 in	0.0060	0.3018	0.1145	0.0130	0.4204	0.1424	0.0018	0.0000	0.0000
R4 out	0.0060	0.2900	0.1264	0.0011	0.4323	0.1424	0.0018	0.0000	0.0000
V1 in	0.0060	0.2900	0.1264	0.0011	0.4323	0.1424	0.0018	0.0000	0.0000
V1 top	0.0084	0.0029	0.1771	0.0016	0.6074	0.2001	0.0026	0.0000	0.0000
C1 in	0.0084	0.0029	0.1771	0.0016	0.6074	0.2001	0.0026	0.0000	0.0000
C1 out	0.0102	0.0005	0.0030	0.0019	0.7404	0.2408	0.0031	0.0000	0.0000
R5 in	0.0102	0.0005	0.0030	0.0019	0.7404	0.2408	0.0031	0.0000	0.0000
R5 out	0.0153	0.0085	0.0000	0.0000	0.7298	0.2433	0.0032	0.0000	0.0000
V2 in	0.0153	0.0085	0.0000	0.0000	0.7298	0.2433	0.0032	0.0000	0.0000
V2 top	0.0154	0.0008	0.0000	0.0000	0.7355	0.2452	0.0032	0.0000	0.0000
Hydrogen	-	-	-	-	-	-	-	-	-
V3 in	0.0154	0.0008	0.0000	0.0000	0.7355	0.2452	0.0032	0.0000	0.0000
V3 top	0.0154	0.0005	0.0000	0.0000	0.7357	0.2452	0.0032	0.0000	0.0000
V4 in	0.0154	0.0005	0.0000	0.0000	0.7357	0.2452	0.0032	0.0000	0.0000
V4 top	0.0154	0.0003	0.0000	0.0000	0.7358	0.2453	0.0032	0.0000	0.0000
V5 in	0.0154	0.0003	0.0000	0.0000	0.7358	0.2453	0.0032	0.0000	0.0000
V5 top	0.0154	0.0002	0.0000	0.0000	0.7359	0.2453	0.0032	0.0000	0.0000
V6 in	0.0154	0.0002	0.0000	0.0000	0.7359	0.2453	0.0032	0.0000	0.0000
V6 top	0.0154	0.0002	0.0000	0.0000	0.7359	0.2453	0.0032	0.0000	0.0000
R6 in	0.0823	0.0001	0.0000	0.0000	0.6462	0.2154	0.0177	0.0000	0.0382
R6 out	0.1232	0.0002	0.0000	0.0000	0.2212	0.0737	0.0265	0.0000	0.5551
V7 in	0.1232	0.0002	0.0000	0.0000	0.2212	0.0737	0.0265	0.0000	0.5551
V7 top	0.2306	0.0000	0.0000	0.0000	0.4925	0.1631	0.0578	0.0000	0.0559
V7 btm	0.0380	0.0004	0.0000	0.0000	0.0057	0.0027	0.0017	0.0000	0.9516
V8 in	0.0380	0.0004	0.0000	0.0000	0.0057	0.0027	0.0017	0.0000	0.9516
V8 top	0.3050	0.0000	0.0000	0.0000	0.0478	0.0224	0.0140	0.0000	0.6109
Ammonia	0.0016	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9979
Purge	0.2404	0.0000	0.0000	0.0000	0.4342	0.1447	0.0520	0.0000	0.1287
Recycle	0.2404	0.0000	0.0000	0.0000	0.4342	0.1447	0.0520	0.0000	0.1287

4.1.3   Important results

The most important results for the standard case, concerning profitability and ammonia production, is presented in table 4.3.

Table 4.3: Important results in the standard case.

Object	Value
Inlet flow	20000 kg/h
Methane out of sec. reformer	56 kmol/h
Hydrogen into synthesis loop	3939 kmol/h
Ammonia	43199 kg/h
Shaft work	30594 kW

4.2   Front-end pressure

In the front-end pressure case the following input data was used: $p_{in} = 50$ bar, $x_{O_2} = 0.21$, Steam/Carbon $= 3.5$, $H_2/N_2 = 3$ and $p_{synthesis} = 235$ bar. Tables of the mole fractions and conditions in and out of the system are presented in appendix A.1.

To find the most profitable inlet pressure a simple optimization equation was used. In the equation the difference in exergy is excluded but later included in the cost estimation. For the front-end pressure case the following equation was used:

$$\Delta \text{Profit} = (\hat{m}_{NH_3} - \hat{m}^*_{NH_3})C_{NH_3} - (W - W^*)C_{el} \qquad (4.1)$$

Here $\hat{m}_{NH_3}$ is ammonia produced in kg/h, C_{NH_3} is the price of ammonia in NOK/kg, W is the shaft work in kWh/h and C_{el} is the price of electricity in NOK/kWh. The * denotes the values for the given variables in the standard case.

Figure 4.1: Graphical representation of additional profit compared to the standard case as a function of inlet pressure.

Table 4.4: Profit analysis of the pressure case. The value p is the inlet pressure which was the adjusted variable. The optimal pressure is marked with bold text.

p [bar]	Shaft work [kW]	Ammonia production [kg/h]	Relative Profit [NOK/h]
60	30590	43190	0
59	30950	43300	149
58	31500	43600	680
57	32090	43910	1222
56	32720	44180	1660
55	33360	44420	2025
54	34070	44670	2392
53	34860	44890	2665
52	35720	45090	2872
51	36700	45260	2973
50	**37840**	**45430**	**3025**
49	39060	45570	2984
48	40520	45700	2848

4.2.1   Important results

The most important results for the front-end pressure case at optimal conditions, concerning profitability and ammonia production, is presented in table 4.5.

Table 4.5: Important results in the front-end pressure case.

Object	Value
Inlet flow	20000 kg/h
Methane out of sec. reformer	13 kmol/h
Hydrogen into synthesis loop	4076 kmol/h
Ammonia	45430 kg/h
Shaftwork	37840 kW

4.3   Hydrogen-nitrogen ratio

In the hydrogen-nitrogen case the following input data is used: p_{in} = 60 bar, x_{O_2} = 0.21, Steam/Carbon = 3.5, H_2/N_2 = 2.6 and $p_{synthesis}$ = 235 bar. Tables of the mole fractions and conditions in and out of the system is presented in appendix A.2.

For the optimization of the hydrogen-nitrogen ratio the same equation as for the optimization of the front-end pressure, equation 4.1, was used.

Figure 4.2: Graphical representation of additional profit compared to the standard case as a function of hydrogen-nitrogen ratio.

Table 4.6: Profit analysis of the hydrogen-nitrogen case. The value H2/N2 is the inlet hydrogen-nitrogen ratio which is the adjusted variable. The optimal ratio is marked with bold text.

H2/N2	Shaftwork [kW]	Ammonia Production [kW]	Relative profit [NOK/h]
3.2	29800	41200	-4948
3.1	30500	42700	-1677
3.0	31100	43500	0
2.9	31500	44000	1041
2.8	3200	44300	1586
2.7	32400	44400	1699
2.6	**32900**	**44500**	**1781**
2.5	33500	44400	1369
2.4	34300	44400	1129

4.3.1   Important results

The most important results for the hydrogen-nitrogen ratio case at optimal conditions, concerning profitability and ammonia production, is presented in table 4.7.

Table 4.7: Important results in the hydrogen-nitrogen ratio case.

Object	Value
Inlet flow	20000 kg/h
Methane out of sec. reformer	21 kmol/h
Hydrogen into synthesis loop	3960 kmol/h
Ammonia	44500 kg/h
Shaftwork	32900 kW

4.4   Steam-carbon ratio

In the steam - carbon case the following input data was used: $p_{in} = 60$ bar, $x_{O_2} = 0.21$, Steam/Carbon = 4.6, $H_2/N_2 = 3$ and $p_{synthesis} = 235$ bar. Tables of the mole fractions and conditions in and out of the system is presented in appendix A.3.

To optimize the steam-carbon ratio a very similar equation as for the nitrogen-hydrogen ratio and inlet pressure were used. In addition a term for the difference in amount of steam were included.

$$\Delta \text{Profit} = (\hat{m}_{NH_3} - \hat{m}_{NH_3}^*) \, C_{NH_3} - (W - W^*) \, C_{el} - (\hat{m}_{steam} - \hat{m}_{steam}^*) \, C_{steam} \qquad (4.2)$$

Where $\hat{m}_{steam}$ is the amount of steam into the plant in kg/h and C_{steam} is the cost of steam in NOK/kg.
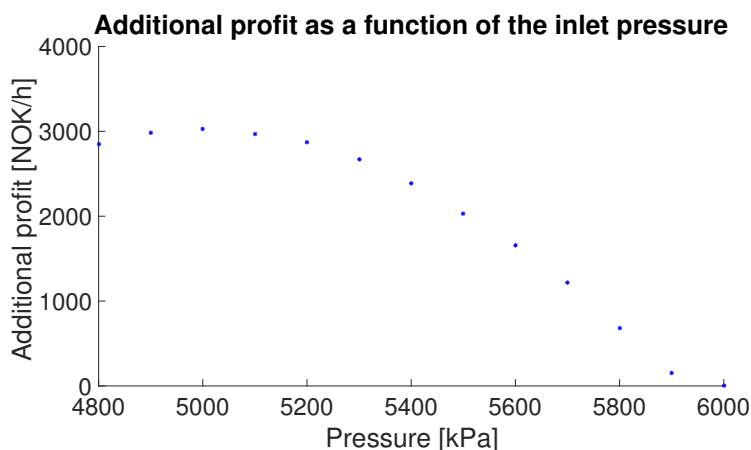

Figure 4.3: Graphical representation of additional profit compared to the standard case as a function of steam-carbon ratio.

Table 4.8: Profit analysis of the steam-carbon ratio case. The amount of steam was the adjusted variable. The optimal ratio is marked with bold text.

Steam/Carbon	Shaftwork [kW]	Ammonia Production [kW]	Steam [ton/h]	Relative profit [NOK/h]
3.0	30019	40914	67.4	-4038
3.5	30958	43199	78.6	0
3.6	31075	43507	80.9	482
3.8	31301	44079	85.4	1347
4.0	31478	44517	89.9	1917
4.2	31603	44889	94.4	2350
4.4	31691	45139	98.9	2661
4.6	**31773**	**45384**	**103.3**	**2661**
4.8	31808	45536	107.8	2611
5.0	31853	45634	112.3	2431
5.2	31883	45770	116.8	2344
5.4	31912	45908	121.3	2261
5.6	31920	45953	125.8	1970

4.4.1 Important results

The most important results for the steam-carbon ratio case at optimal conditions, concerning profitability and ammonia production, is presented in table 4.9.

Table 4.9: Important results in the steam carbon ratio case.

Object	Value
Inlet flow	20000 kg/h
Methane out of sec. reformer	21 kmol/h
Hydrogen into synthesis loop	4067 kmol/h
Ammonia	45384 kg/h
Shaftwork	31773 kW

4.5 Mole fraction oxygen by membrane

In the mole fraction oxygen by membrane case the following input data was used: $p_{in} = 60$ bar, $x_{O_2} = 0.235$, Steam/Carbon $= 3.5$, $H_2/N_2 = 3$ and $p_{synthesis} = 235$ bar. Tables of the mole fractions and conditions in and out of the system is presented in appendix A.4.

To optimize the mole fraction of oxygen a very similar equation as for the nitrogen-hydrogen ratio and inlet pressure were used. In addition a term for the cost of producing oxygen by separation of air were included.

$$\Delta \text{Profit} = (\hat{m}_{NH_3} - \hat{m}^*_{NH_3})C_{NH_3} - (W - W^*)C_{el} - (\hat{n}_{O_2} - \hat{n}^*_{O_2})C_{O_2,\text{membrane}} \qquad (4.3)$$

Here $\hat{n}_{O_2}$ is the amount of pure oxygen added to the air stream in kmol/h and C_{O_2} is the cost of producing the oxygen through membrane separation of air in NOK/kmol.
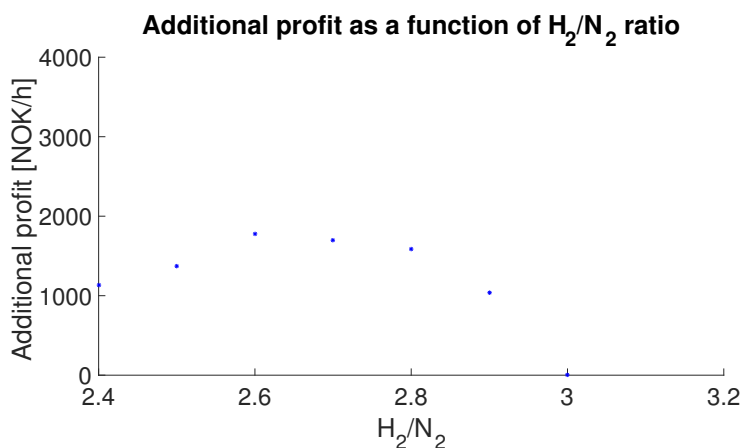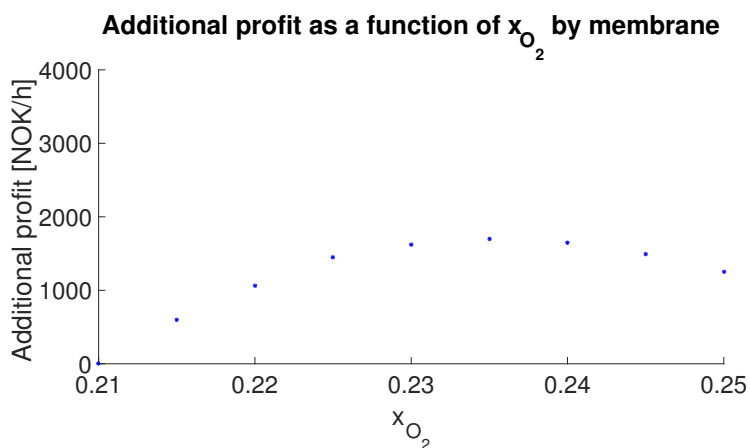

Figure 4.4: Graphical representation of additional profit compared to the standard case as a function of the mole fraction of oxygen by production of oxygen through membrane separation of air.

Table 4.10: Profit analysis of the mole fraction oxygen by membrane separation of air case. The amount of additional O_2 was the adjusted variable. The optimal mole fraction is marked with bold text.

x_{O_2}	Shaftwork [kW]	Ammonia Production [kW]	Additional O2 [kmol/h]	Relative profit [NOK/h]
0.210	30970	43210	0	0
0.215	31070	43500	11.1	596
0.220	31160	43730	22.2	1056
0.225	31240	43930	33.8	1447
0.230	31280	44030	45.5	1618
0.235	**31300**	**44090**	**57.5**	**1700**
0.240	31290	44090	69.6	1652
0.245	31260	44040	82	1492
0.250	31210	43950	94.5	1246

4.5.1   Important results

The most important results for the mole fraction oxygen by membrane case at optimal conditions, concerning profitability and ammonia production, is presented in table 4.11.

Table 4.11: Important results in the mole fraction oxygen by membrane case.

Object	Value
Inlet flow	20000 kg/h
Methane out of sec. reformer	20 kmol/h
Hydrogen into synthesis loop	3966 kmol/h
Ammonia	44090 kg/h
Shaftwork	31300 kW

4.6   Mole fraction oxygen by electrolysis

In the mole fraction oxygen by electrolysis case the following input data was used: $p_{in} = 60$ bar, $x_{O_2} = 0.231$, Steam/Carbon $= 3.5$, $H_2/N_2 = 3$ and $p_{synthesis} = 235$ bar. Tables of the mole fractions and conditions in and out of the system is presented in appendix A.5.

To optimize the mole fraction of oxygen a very similar equation as for the nitrogen-hydrogen ratio and inlet pressure were used. In addition a term for the cost of producing oxygen by electrolysis of water.

$$\Delta\text{Profit} = (m_{NH_3} - m_{NH_3}^*)\, C_{NH_3} - (W - W^*)C_{el} - (n_{O_2} - n_{O_2}^*)\, C_{O_2,\text{electrolysis}} \qquad (4.4)$$

Here n_{O_2} is the amount of pure oxygen added to the air stream in kmol/h and C_{O_2} is the cost of producing the oxygen through electrolysis of water in NOK/kmol.
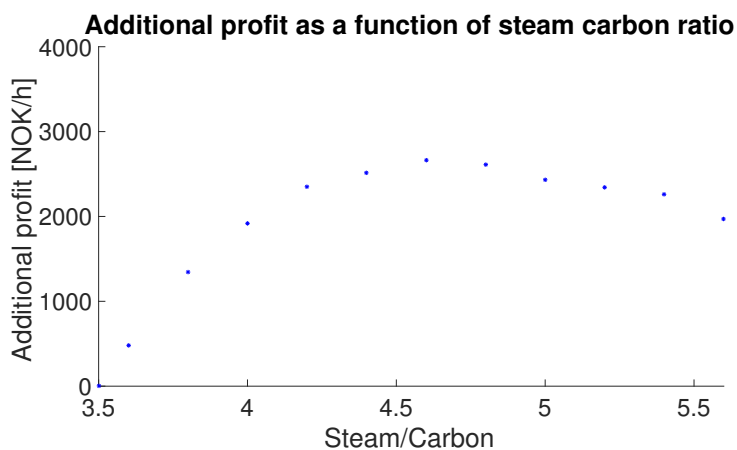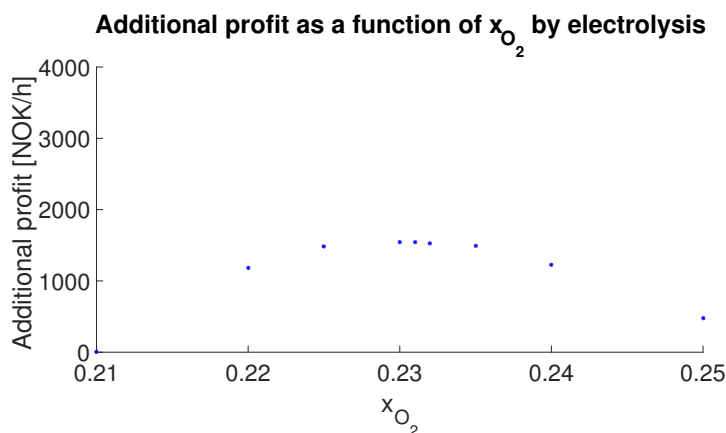

Figure 4.5: Graphical representation of additional profit compared to the standard case as a function of the mole fraction of oxygen by production of oxygen by electrolysis.

Table 4.12: Profit analysis of the mole fraction oxygen by electrolysis case. The amount of additional O_2 was the adjusted variable. The optimal mole fraction is marked with bold text.

x_{O_2}	Shaftwork [kW]	Ammonia Production [kW]	Additional O2 [kmol/h]	Relative profit [NOK/h]
0.21	30941	431780	0	0
0.22	31813	44318	22.2	1182
0.225	32139	44757	33.8	1483
0.23	32382	45087	45.6	1540
0.231	**32460**	**45155**	**48**	**1547**
0.232	32511	45209	50.4	1529
0.235	32643	45380	57.6	1496
0.24	32869	45576	69	1226
0.25	33290	45887	94.8	479

4.6.1   Important results

The most important results for the mole fraction oxygen by electrolysis case at optimal conditions, concerning profitability and ammonia production, is presented in table 4.13.

Table 4.13: Important results in the mole fraction oxygen by membrane case.

Object	Value
Inlet flow	20000 kg/h
Methane out of sec. reformer	20 kmol/h
Hydrogen into synthesis loop	4060 kmol/h
Ammonia	45155 kg/h
Shaftwork	32460 kW

4.7   Summary and comparison

To summarize the given results, the important results in the previous subsections is given in one table. In addition all the plots are given in one figure to illustrate the difference in magnitude of profitability between each of the cases.
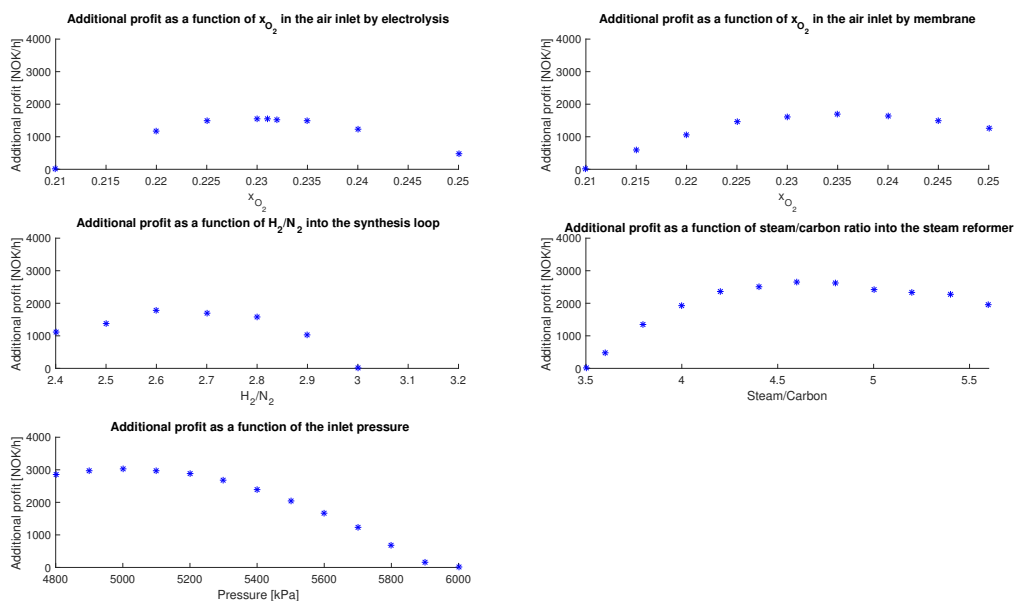
Figure 4.6: Graphical representation of additional profit compared to the standard case for all the cases given in this section 4.

Table 4.14: A summary of all the key results in all six cases gathered in one table.

Case	Ammonia [kg/h]	Shaft work [kW]	Steam [ton/h]	n_{R2,out,CH_4} [kmol/h]	$n_{V6_{top,H_2}}$ [kmol/h]	Relative profit [NOK/h]
Standard	43199	30594	78.6	56	3939	0
Front-end pressure	45430	37840	78.6	13	4076	3025
Hydrogen-nitrogen	44500	32900	78.6	21	3960	1781
Steam-carbon	45384	31773	103.3	21	4067	2661
Membrane	44090	31300	78.6	20	3966	1700
Electrolysis	45155	32460	78.6	20	4060	1547

5   Cost estimations

In this section the cost estimations will be described. The sizing of the equipment is based on the model of the ammonia factory, NII, Herøya, Porsgrunn. Units from Aspen HYSYS simulations were used to estimate the cost of the major equipment. Further on, the calculated cost of equipment was used in the calculations of the total capital

investment, composed of fixed and working capital. Variable and fixed costs of production are included as well as annual sale income. Calculations is based on equations from Sinnot & Towler (2009) [15].

The major equipment is set to be compressors, heat exchangers, reactors, separators, absorbers and pumps. The number of units varies slightly from case to case.

The purchased equipment cost on a US Gulf Coast basis (Jan. 2007) can be calculated as in equation 5.1:

$$C_{\text{e}} = a + bS^{\text{n}} \tag{5.1}$$

Where a and b are cost constants, S is the size parameter and n is the exponent for that type of equipment. The values for a, b and n are given in table 6.6 in Sinnot & Towler [15]. The sizing value, S, is both calculated and gathered from Aspen HYSYS. Values in table 6.6 are only valid between the lower, S_{lower}, and upper, S_{upper}, values of S as indicated. All the values were calculated on a US Gulf coast basis from January 2007. At this year the CE index (CEPCI) was 509.7. To approximate the price in 2016 , all purchased equipment cost had to be multiplied by the ratio of cost in year 2016 and cost in year 2007 as given in equation 5.2[16].

$$I_{2016,2007} = \frac{I_{2016}}{I_{2007}} = \frac{556.8}{509.7} \tag{5.2}$$

This is important to include because all cost-estimating methods use historical data and the prices of the materials and the cost of labour are subject to inflation. This CE index for 2016 is therefore to update old cost data and to forecast the future cost of the plant.

After multiplying with the ratio of the CE index, the purchased equipment cost had to be converted from US dollars to NOK. The exchange rate per 25th of october 2016, was 8.26 NOK/US Dollar [17].

5.1   Compressors

For estimating the cost of the compressors, values for centrifugal compressors were used. The standard, hydrogen-nitrogen ratio, steam-carbon ratio, front-end pressure and the mole fraction by membrane case have 10 compressors. They are named K-1, K-2, K-3, K-4, K-5, K-6, K-7, K-8, K-9 and K-13 in flowsheet, figure 3.1. In the electrolysis case the simulation had 13 compressors. They are named from K-1 to K-13 as shown in figure 3.1.

The calculated cost for one compressor is stated in equation 5.3;

$$C_e = 490000 + 16800 \ W^{0.6} \tag{5.3}$$

The sizing factor is W, duty [kW] of the compressor, which is given in the Aspen HYSYS simulation. This estimated cost for the compressors are given for compressors in carbon steel, so C_e were multiplied by the material cost factor for stainless steel which is 1.3 [15]. The estimated cost of all the compressors (in ss 304) in all six cases are given in table 5.1.

Table 5.1: The table is showing the calculated cost of all the compressors for the six cases.

Case	Cost of compressors [NOK (2016)]
Standard	256 217 269
Hydrogen-nitrogen ratio	265 355 329
Steam-carbon ratio	259 224 869
Front-end pressure	266 420 296
Mole fraction oxygen by membrane	257 810 567
Mole fraction oxygen by electrolysis	290 898 398

As expected, the purchased cost of the compressors in the electrolysis case is higher than the costs in the other cases. This is due to the fact that it needed 13 compressors.

5.2 Reactors

For estimating the cost of the reactors, values were found for jacketed, agitated reactors where the price estimate was given in 304 stainless steel. The cost estimation was calculated from equation 5.4;

$$C_e = 53000 + 28000 \ V^{0.8} \tag{5.4}$$

where V is the reactor volume. The reactor volume for the secondary reformer, R-2, the two water-gas shift reactors, R-3 and R-4, the methanation reactor, R-5, and the synthesis reactor, R-6, were approximated using residence time for each reactor[18]. The residence time for R-6, the ammonia synthesis reactor, was found to be 33 s and for the other reactors it was assumed a residence time of 5 s[19]. To estimate a reactor volume with residence time equation 5.5 was used:

$$V = \frac{\hat{V}\tau}{\phi} \tag{5.5}$$

where $\hat{V}$ is the volume flow into the reactor, τ the residence time and the void fraction, ϕ. The void fraction, ϕ, of the reactors was assumed to be 0.45 for every case. The cost of the reactors where residence time was used to calculate volume are listed in table 5.2.

Table 5.2: The table is showing the calculated cost of all the reactors except the primary reformer for the six simulations. All costs in NOK per 2016.

Case	Cost of reactor R-2, R-3, R-4, R-5 and R-6 [NOK (2016)]
Standard	31 024 848
Hydrogen-nitrogen ratio	33 332 611
Steam-carbon ratio	34 091 682
Front-end pressure	44 241 538
Mole fraction oxygen by membrane	31 352 414
Mole fraction oxygen by electrolysis	31 503 967

5.2.1 Primary reformer

For the estimation of the cost for the primary reformer, equation 5.4 was used. As "the high alloy reformer tubes are expensive and account for a large part of the reformer costs", the volume of the reformer tubes was estimated for the sizing parameter [20]. The length of each tube was assumed to be 10 m, and from this the diameter, volume and number of reformer tubes was estimated, as shown in appendix B.1. The estimated volume of tubes was assigned to the standard case so it would work as a reference volume. Thereafter each case was scaled in comparison to the standard case where the scaling factor was inlet volume flow of each case, divided by inlet volume flow of standard case. The tubes were assumed to be made of inconel which results in a new material factor to be multiplied with the price.

Table 5.3: The table is showing the calculated cost of the primary reformer, R1, for all six simulations. All costs are in NOK per 2016

Case	Cost of reactor R-1 [NOK (2016)]
Standard	7 082 062
Hydrogen-nitrogen ratio	7 082 062
Steam-carbon ratio	8 303 497
Front-end pressure	9 966 787
Mole fraction oxygen by membrane	7 082 062
Mole fraction oxygen by electrolysis	7 082 062

5.3 Exchangers

The heat exchangers were modeled as heaters and coolers in Aspen HYSYS for all the six cases. They are named from H-1 to H-20 in figure 3.1. In this estimation of the purchased costs it was assumed "U-tube shell and tube exchangers" where the area, A, is needed as the sizing parameter. To calculate the area, equation 5.6 is used [21]:

$$Q = UA\Delta T_{\text{AM}} \tag{5.6}$$

A [m^2] is the heat transfer area. The value of Q [W] is the duty of the cooler/heater and U [W/m^{2}K] is the coefficient of the heat transfer. U is assumed to be 400 W/m^{2}K, which is a typical value for industrial heat exchangers at these conditions. Δ T$_{AM}$ [K] is gathered from the temperature in to the cooler/heater, T$_1$, and temperature out of the cooler/heater, T$_2$ as in appendix B.2. T$_{AM}$ is the arithmetical mean temperature.

The purchased costs for the exchangers is given in equation 5.7.

$$C_e = 24000 + 46 \; A^{1.2} \tag{5.7}$$

This cost estimate is given in carbon steel, so C$_e$ had to be multiplied by the material cost factor for stainless steel 304. This factor, f$_m$ is 1.3. The purchased cost for all the exchangers in stainless steel 304 for all the six simulations are given in table 5.4.

Table 5.4: The table is showing the calculated cost for all the heat exchangers in the six cases.

Case	Cost of exchangers [NOK (2016)]
Standard	18 440 483
Hydrogen - Nitrogen ratio	19 715 408
Steam-Carbon ratio	21 179 646
Front-end pressure	18 540 594
Mole fraction oxygen by membrane	18 535 622
Mole fraction oxygen by electrolysis	18 651 577

5.4   Separators

The separation of liquids droplets and vapour streams is analogous to the separation of solid particles and, with the possible exception of filtration, the same techniques and equipment can be used [15]. It is often enough to use gravity settling in a vertical separating vessel. The settling velocity of the liquid droplets had to be estimated by equation 5.8:

$$u_t = 0.07 \sqrt{\frac{(\rho_L - \rho_V)}{\rho_V}} \tag{5.8}$$

where u$_t$ is the settling velocity [m/s], ρ_L is the density of the liquid [kg/m^3] and ρ_V is the density of the vapour [kg/m^3]. These values were gathered from the simulations. In these separators, demister pads were used, so it was not necessary to multiply u$_t$ by 0.15 to provide a margin of safety and to allow for flow surges. To get the desired value of the height of the separators, the minimum diameters were estimated by equation 5.9:

$$D_V = \sqrt{\frac{4\hat{V}_V}{\pi u_s}} \tag{5.9}$$

This diameter must be large enough to slow the gas down at which the droplets will settle out. D_V is here the minimum vessel diameter [m], $\hat{V}_V$ is the volumetric flow rate of vapour [m^3/s] from simulations, and $u_s = u_t$ if a demister pad is used. The diameters were rounded to the nearest standard vessel size, so standard vessel closures could be used. The liquid volumetric flow rate [m^3/s] from the simulations were used to find the amount of liquid volume held in the vessel, h_L as in appendix B.5. The hold up time were set to 10 minutes. The total height of the separators are given in equation 5.10:

$$h_{tot} = h_L + \frac{D_V}{2} + D_V + 0.4 \tag{5.10}$$

The shell mass of the separators are calculated as in equation 5.11:

$$m_{shell} = \pi \; D_V \; h_{tot} \; t_w \; \rho \tag{5.11}$$

where t_w is the wall thickness [m], calculated in appendix B.5, and ρ is the density [kg/m^3] of the metal which is 8030 kg/m^3 for stainless steel 304 [22]. The estimated purchased costs of the eight separators are calculated as 5.12:

$$C_e = 15000 + 68 \; m_{shell}^{0.85} \tag{5.12}$$

The total purchased costs for the eight separators, V-1 to V-8, are given in table 5.5 for the different cases.

Table 5.5: The table is showing the calculated cost for all the eight separators for the six cases. Costs given in NOK per 2016

Case	Cost of separators [NOK (2016)]
Standard	16 228 279
Hydrogen - Nitrogen ratio	17 779 010
Steam-Carbon ratio	16 670 980
Front-end pressure	15 740 632
Mole fraction oxygen by membrane	15 856 075
Mole fraction oxygen by electrolysis	15 918 984

5.5 Absorbers

Four absorbers were simulated in Aspen HYSYS. 15 stages were needed to get the desired amount of carbon dioxide out. Assuming 0.5 m between the stages in addition to the bottom and top space, gave a height of the absorbers to be 9.5 m. The diameter was assumed to be 1.5 m which is half of 3 meter, as on NII (Herøya, Porsgrunn). This assumption was based on the fact that the simulations only have 15 stages, and the actual absorbers on NII(Herøya, Porsgrunn) have 72 stages.

The purchased costs of the sieve trays were calculated as in equation 5.13. The sizing parameter is the diameter, D [m].

$$C_e = 110 + 380 \ D^{1.8} \tag{5.13}$$

The mass of a vertical pressure vessel, in stainless steel 304, had to be calculated to get the rest of the purchased costs of the absorbers. Operating pressure, shear stress and diameter were used to calculate the wall thickness. The wall thickness and the height were further used to calculate the mass [kg] as in appendix B.4. Calculated purchased cost of the pressure vessel is given in equation 5.14:

$$C_e = 15000 + 68 \ m^{0.85} \tag{5.14}$$

where m [kg] is the sizing parameter. Calculated purchased cost of the sieve trays plus the pressure vessel gave the total cost of the absorbers, as given in table 5.6.

Table 5.6: The table is showing the calculated cost for the four absorbers for the six cases. The costs are given in NOK per 2016

Cases	Cost of absorbers [NOK (2016)]
Standard	6 196 145
Hydrogen - Nitrogen ratio	6 196 145
Steam-Carbon ratio	6 196 145
Front-end pressure	4 208 699
Mole fraction oxygen by membrane	6 196 145
Mole fraction oxygen by electrolysis	6 196 145

5.6 Pumps

The estimation of the purchased costs of the pumps is calculated for four pumps. Only one of them are showed in figure 3.1, but four are modelled. The calculation is the same for all six cases, but the different sizing values for flow and power are different. To calculate the cost of the pumps it was assumed that they are single-stage centrifugal. The lower sizing value is $S_{lower} = 0.2$ L/s and the upper sizing value $S_{upper} = 126$ L/s. The upper sizing value is too low for the flows in the model. The model flows are over 600 L/s, but it was still assumed that the cost estimation could be carried out by the given values. Calculated purchased costs for the single-stage centrifugal is given in equation 5.15:

$$C_e = 6900 + 206 \ q^{0.9} \tag{5.15}$$

The sizing value, q, is gathered from the HYSYS model. The motors used for the pumps are called explosion proof motors [kW], and the powers are taken from the simulations and substituted for P in equation 5.16. Estimated purchased costs of the motors are:

$$C_e = -950 + 1770\ P^{0.6} \tag{5.16}$$

The total price for one pump were the cost of the single-stage centrifugal and the explosion proof motor. To get the estimated purchased cost for the pumps in stainless steel 304, C_e were multiplied by material cost factor at 1.3. Calculated purchased costs for all four pumps in the six different cases are given in table 5.7.

Table 5.7: The table is showing the calculated cost for the four pumps for the six cases. Costs are given in NOK per 2016.

Case	Cost of pumps [NOK (2016)]
Standard	10 700 271
Hydrogen - Nitrogen ratio	10 975 461
Steam-Carbon ratio	10 855 903
Front-end pressure	15 568 505
Mole fraction oxygen by membrane	10 747 187
Mole fraction oxygen by electrolysis	10 763 649

The front-end pressure case have higher costs of pumps than that of the others.

5.7   Total investment costs

Total investment costs consist of total fixed capital and working capital.

5.7.1   Total fixed capital costs

To calculate the total fixed capital costs, equation 5.17 is used:

$$C_{FC} = C(1 + OS)(1 + D\&E + X) \tag{5.17}$$

The explanation of the symbols are given in table 5.8. C is the sum of C_{SS} and C_{NI} from equation 5.18 and 5.19. This is referred to as inside battery limits, ISBL, the cost of procuring and installing all the process equipment. To calculate the value of C_{SS} for all the equipment in material 304 stainless steel, equation 5.18 is used;

$$C_{SS} = \sum_{i=1}^{i=M} C_{e,i,SS}\ \left((1 + f_p) + (f_{er} + f_{el} + f_i + f_c + f_s + f_l)/f_{SS}\right) \tag{5.18}$$

M is the total number of components being recalculated into stainless steel costs. The other symbols in equation 5.18 and 5.17 are listed in table 5.8. From this equation it can be seen that the piping will be in stainless steel 304. The other equipments like electrical, instrumentation etc. are divided by material factor, $f_{m,SS} = 1.3$.

The only equipment that should not be in stainless steel, is the primary reformer, R-1 in flowsheet, figure 3.1. The material of this reactor is nickel and inconel. The costs of the primary reformer, $C_{e,i,NI}$ is given in equation 5.19:

$$C_{NI} = \sum_{i=1}^{i=M} C_{e,i,NI} \left((1 + f_p) + (f_{er} + f_{el} + f_i + f_c + f_s + f_l)/f_{NI}\right) \tag{5.19}$$

It is important to notice that the material factor for nickel and inconel is $f_{m,NI}=1.7$. The other parameters are given in table 5.8.

Table 5.8: The table are showing parameters which is of process type were fluids are used. These parameters are used in 5.17, 5.18

Major equipment, total purchase cost	C_e value	Comment
f_{er}	0,3	Equipment erection
f	0,8	Piping
f_i	0,3	Intrumentation and control
f_{el}	0,2	Electrial
f_c	0,3	Civil
f_s	0,2	Structures and buildings
f_l	0,1	Lagging and paint
OS	0,3	Offsites
D&E	0,3	Design and Engeneering
X	0,1	Contigency

The total value of C is now the sum of C_{SS} and C_{NI}. C is then used in equation 5.17 to get to total fixed capital costs. Table 5.9 is showing the calculated total fixed investment costs in NOK per 2016.

Table 5.9: The table is showing the calculated total fixed capital costs for the six simulations. The costs are given in NOK per 2016

Simulation	C_{FC} [NOK (2016)]
Standard	1 807 810 606
Hydrogen - Nitrogen ratio	1 883 976 969
Steam-Carbon ratio	1 862 923 600
Front-end pressure	1 957 264 945
Mole fraction oxygen by membrane	1 816 663 189
Mole fraction oxygen by electrolysis	1 991 727 325

5.7.2   Working capital

Working capital is the additional money needed, in addition to the cost of building the plant, to start the plant up and run it until it starts earning income. It includes the cost of raw material inventory (2 weeks delivered costs of raw materials), the value of the product (2 weeks cost of production), cash on hand, accounts receivable etc. Working capital can be calculated by the cost of production. It can be assumed 5% of the fixed capital, calculated in equation 5.17. Table 5.10 gives the working capital for the six case.

Table 5.10: The table is showing the working capital for the six cases. The costs are given in NOK per 2016

Simulation	Working capital [NOK (2016)]
Standard	90 390 530
Hydrogen-nitrogen ratio	94 198 848
Steam-carbon ratio	93 146 179
Front-end pressure	97 863 247
Mole fraction oxygen by membrane	90 833 159
Mole fraction oxygen by electrolysis	99 586 366

5.8   Variable costs

Variable costs of production are costs that are proportional to the plant output. It was assumed 352 production days per year. In most of the cases, variable costs includes cost of steam, compressor costs and cost of natural gas feed. In the membrane and the electrolysis case, cost of extra oxygen are included. The production costs which is not included is water and waste disposal costs. These are expenses which are excluded in the calculated working capital, but in reality will affect the costs. To simplify the heat integration calculation (utility, fired heat, cooling, electricity), the exergy were calculated instead. Exergy will be further explained in section 5.10. The total variable costs are presented in table 5.15.

5.8.1   Cost of steam

The steam cost estimation is here referred to as extra steam supplied to the plant. Molar flows of steam, $\hat{n}$ [kmol/h] from Aspen HYSYS were used to find the mass flows, $\hat{m}$ [ton/h]. The cost of the steam were calculated as in equation 5.20:

$$C_{steam} = \hat{m}\frac{ton}{h} \cdot 8.76\frac{\pounds}{ton}\ 10.46\frac{NOK}{\pounds} \tag{5.20}$$

where MP, medium pressure, steam cost 8.76 £/ton [15].The definition of MP steam is 20 bar at 212°C and high pressure steam, HP, 40 bar at 250°C. The estimated prices for steam production in the six cases are given in table 5.11.

Table 5.11: The calculated cost of producing steam used in the production. Cost is given for all the the six cases in NOK per 2016.

Cases	Cost of steam [NOK/year]
Standard	60 791 139
Hydrogen-nitrogen ratio	60 791 139
Steam-carbon ratio	79 907 674
Front-end pressure	60 791 139
Mole fraction oxygen by membrane	60 791 139
Mole fraction oxygen by electrolysis	60 791 139

5.8.2   Compressor costs

In the simulations adiabatic compressors were used so all supplied work is added to the internal energy of the gas. The supplied work is electricity. Total compression work [kW] were gathered from Aspen HYSYS to find the cost of the electricity [23].

The estimated price for electricity into the compressors in the six cases are given in table 5.12.

Table 5.12: The table gives calculated cost of electricity used to drive the compressors. Cost is given for all the the six cases.

Cases	Cost of compressor electricity [NOK/year]
Standard	77 527 296
Hydrogen-nitrogen ratio	82 469 376
Steam-carbon ratio	79 428 096
Front-end pressure	95 698 944
Mole fraction oxygen by membrane	78 414 336
Mole fraction oxygen by electrolysis	81 607 680

5.8.3   Cost of methane, CH_4

Methane feed to the plant was set as a basis of 20 ton/h for all six simulations. To calculate the cost of methane, natural gas prices were used [14]. The cost of methane as feed were calculated to be 23139.8 NOK/h. This price was the same for all six simulations.

To heat up the primary reformer, some extra methane had to be added. The thought was to replace electrical heating with thermal heating using the methane and hydrogen from the purge, along with an extra amount of methane so no electrical heating was necessary. The cost of additional methane needed was calculated and the hot fluegas out of the reformer were added as extra income in the exergy balance.

The calculated amount of extra methane, in addition to the methane in the feed gives the total cost of methane. The calculations for extra methane is shown in appendix B.9.

The results are given in table 5.13.

Table 5.13: The table gives calculated cost for methane in the feed and the extra methane needed to fire the primary reformer. Cost is given for all the the six cases.

Case	Cost of CH_4 [NOK/year]
Standard	230 356 534
Hydrogen-nitrogen ratio	239 942 001
Steam-carbon ratio	247 608 618
Front-end pressure	245 841 786
Mole fraction oxygen by membrane	238 912 011
Mole fraction oxygen by electrolysis	238 442 692

5.8.4   Cost of oxygen

In case 3.1.4 and 3.1.5, some extra oxygen is used to increase the hydrogen production. The calculated amount of oxygen were calculated in appendix B.7. Table 5.14 displays the amount of oxygen [kmole/year] and the costs.

Table 5.14: The table gives calculated amount of oxygen [kmole/year] and cost needed to produce hydrogen from membrane technology and electrolysis.

Case	Amount of O_2 [kmole/year]	Cost of O_2 [NOK/year]
Mole fraction oxygen by membrane	473 088	2 001 162
Mole fraction oxygen by electrolysis	405 335	20 714 209

5.8.5   Variable costs total

The total variable costs are given in 5.15. Steam-carbon case is the most expensive, and the standard has the lowest variable costs.

Table 5.15: The table gives calculated variable costs in NOK per year.

Case	Variable costs [NOK/year]
Standard	368 674 970
Hydrogen-nitrogen ratio	383 202 516
Steam-carbon ratio	406 944 389
Front-end pressure	402 331 870
Mole fraction oxygen by membrane	378 117 487
Mole fraction oxygen by electrolysis	401 555 721

5.9   Fixed costs of production

Fixed costs of production are costs that are incurred regardless of the plant operating rate or output. If the plant has a shutdown, these costs still have to be paid for. These costs includes operating labours, supervision, direct salary overhead, maintenance, property taxes, rent of land etc.

Operator salaries varies by seniority. The salaries are also dependent on location. As an assumption it can be estimated an average salary for this case, 500 000 NOK/year per shift. Total expenses in operator salaries were calculated to be 7 441 891 NOK/year if number of operators are 15, which is an assumption. Operator salaries would not vary from case to case.

Supervision is usually taken as 25 % of operating labour. The cost of supervision will then be 1 860 472 NOK/year. Direct salary overhead can also be taken into account. This includes costs of fringe benefits, payroll taxes and health insurances. This is about 40-50% of operating salaries plus supervision. Here it was assumed as 40% of operating salaries resulting in direct salary overhead at 4 837 229 NOK/year .

In addition, other expenses such as maintenance and property taxes, were included. Maintenance includes both materials and labour. It can be calculated as 3-5% of ISBL. Here, it was assumed that maintenance is 3% of ISBL investment. Property taxes and incurance are assumed 1% of ISBL fixed capital. Other labour costs such as rent of land, general plant overhead, capital charges, sales and marketing costs are not included. This is because they will be about the same for all the six cases. All fixed costs are summed up an given for all six cases in table 5.16.

Table 5.16: Fixed production costs for all six cases.

Cases	Fixed costs of production [NOK/year]
Standard	53 871 694
Hydrogen-nitrogen ratio	55 545 681
Steam-carbon ratio	55 082 969
Front-end pressure	57 156 405
Mole fraction oxygen by membrane	54 066 257
Mole fraction oxygen by electrolysis	57 913 820

5.10   Annual sale income

Annual sale income is mainly the price of selling the product, but exergy available at the plant can also be seen as an income.

5.10.1   Ammonia, NH$_3$

Ammonia is the main product in this process. Producing a lot of ammonia at great prices are beneficial. The ammonia price were found to be about 2.23 NOK/kg$_{\text{NH}_3}$ [13]. The calculated prices are given in table 5.17.

Table 5.17: The table gives calculated price for the ammonia in NOK per year.

Case	Price for Ammonia [NOK/year]
Standard	814 783 499
Hydrogen-nitrogen ratio	838 359 410
Steam-carbon ratio	853 636 601
Front-end pressure	856 654 317
Mole fraction oxygen by membrane	831 569 548
Mole fraction oxygen by electrolysis	851 561 921

In the front-end pressure case, most NH$_3$ were produced, which achieves a higher price.

5.10.2   Exergy analysis

In estimating the working capital, utility costs, fired heat, cooling and electricity have to be calculated. As a simplification, the exergy takes these into account.

Exergy is defined as the maximal work you can take out at a given state change compared to the surroundings at given temperature, T$_0$ [B.6].

To calculate the available energy that can be taken out of the process, the Carnot efficiency, T$_{\text{H,lm}}$ and the exergy were calculated as equations B.20 B.21 and B.32 in appendix B.6. The exergy analysis were conducted on all heaters/coolers (H-1 to H-21) and the primary reformer, R-1. The other reactors were assumed to be taken into account when analyzing the coolers and heaters.

The exergy calculated for the primary reformer, R-1, were conducted from properties of the fluegas. Fluegas is the product of the combustion in the primary reformer. The flue gas was assumed to be heat exchanged after R-1. Hot temperature in, T$_{\text{H,in}}$= 760 °C, and hot temperature out, T$_{\text{H,out}}$ = 220 °C, were used to find T$_{\text{H,lm}}$ as in appendix B.11. These temperatures were set equal to the basis, NII, on Herøya. The duty of the exchanger was computed as in equation 5.21:

$$Q = \hat{n}_{\text{fluegas}} c_{\text{p,avg}} \left(T_{\text{H,in}} - T_{\text{H,out}} \right) \tag{5.21}$$

where $\hat{n}_{\text{fluegas}}$ is the calculated molar flow [mole/h] of fluegas. Then molar flow, $\hat{n}_{\text{fluegas}}$, consist of molar flows of nitrogen, argon, water and carbon dioxide. c$_{\text{p,avg}}$ is the average heat capacity [kWh/K*mol] to the fluegas at a given temperature. The duty [kWh], Q, is multiplied by the carnot efficiency to find the theoretical work that can be taken out from the fluegas as in appendix B.20.

To estimate how much electricity this exergy were equivalent, the exergy were multiplied by an energy conversion efficiency. The efficiency of an energy conversion device is a quantitative expression of the balance between energy input and energy output [24]. It is defined as equation 5.22:

$$\text{Device efficiency} = \frac{\text{Useful energy input}}{\text{Energy input}} \qquad (5.22)$$

For thermal/chemical energy to electrical energy, the conversion efficiency is about 60% [25]. After calculating the amount of electricity [kWh] needed, the price [NOK/h] were found for the electricity. The cost of the electricity "produced" at the plant minus the electricity needed gave for all the simulations positive numbers. The calculated amount of money one can get from the process is given in table 5.18

Table 5.18: The table gives calculated price for the exergy available at the plant per year.

Case	Money available from exergy [NOK/year]
Standard	103 324 834
Hydrogen-nitrogen ratio	115 044 304
Steam-carbon ratio	124 947 963
Front-end pressure	111 787 226
Mole fraction oxygen by membrane	111 231 119
Mole fraction oxygen by electrolysis	111 989 246

5.10.3   Total income

Annual sale income are given in table 5.19. The income consist of selling the product, ammonia, and the available work calculated from exergy analysis.

Table 5.19: The table gives calculated income in NOK per 2016. Income is from selling ammonia and available work from exergy

Case	Income [NOK/year]
Standard	918 108 334
Hydrogen-nitrogen ratio	953 403 716
Steam-carbon ratio	978 584 565
Front-end pressure	968 441 544
Mole fraction oxygen by membrane	942 800 668
Mole fraction oxygen by electrolysis	963 551 167

5.11   Annual operating expenses

Total amount expenses are given in table 5.20. The expenses consist of the fixed costs of production and the variable costs of production. The calculated amounts shows that the steam-carbon case is the most expensive considering only the operating expenses. The less expensive case is the membrane case.

Table 5.20: The table gives calculated expenses in NOK per 2016.

Simulation	Expenses [NOK/year]
Standard	422 546 665
Hydrogen-nitrogen ratio	438 748 197
Steam-carbon ratio	462 027 358
Front-end pressure	459 488 275
Mole fraction oxygen by membrane	432 183 744
Mole fraction oxygen by electrolysis	459 469 541

6   Investment analysis

The profitability of the different cases is based on the total capital cost, total income and the expenses per year. The net present value, NPV, was used to find the internal rent of return, IRR.

6.1   Method of evaluation

The method that was chosen to evaluate the profitability of the different cases was the internal rate of return. The IRR method was chosen because when comparing cases, or projects, with different investment costs, the IRR method is more accurate than the net present value. Also both the IRR and NPV method takes the time value of money into account, as opposed to the return of investment method, ROI. The project with the highest IRR always provides the best "bank for the buck"[15]. IRR should also be higher than the capital costs, at 15%. IRR was calculated setting the NPV in equation 6.1 to zero.

IRR was calculated by finding an interest rate that makes the cumulative NPV equal to zero. IRR is the maximum interest rate a project can pay and still break even at the end of the projects life span. The life span of the projects was set to 10 years. The NPV equation 6.1 is shown below.

$$NPV = CF_0 + \sum_{n=1}^{10} \frac{\text{CF}_n}{(1+\text{i})^n}, \ CF_0 = -I - WC \tag{6.1}$$

Where I is the total capital cost and WC the working capital. In order to find IRR, the cashflow, CF_n, had to be found first. All of the calculations for finding IRR were inserted in excel spreadsheet, appendix B.10. In the spreadsheet, the depreciation was first calculated with the declining balance depreciation method. The depreciation factor was set to 20%, then it was calculated over 10 years as described in equation 6.2

$$D = \sum_{n=1}^{10}(0.2(1-0.2)^{n-1}I) = \sum_{n=1}^{10} D_n \qquad (6.2)$$

The tax percentage was to be 28%, which was used on the gross profit minus the depreciation. The gross profit, or GP, is the annual sales income minus the annual service expenses. Equation 6.3 shows how the taxation, T, was calculated.

$$T = \sum_{n=1}^{10}(GP - D_n)0.28 = \sum_{n=1}^{10} T_n \qquad (6.3)$$

After the tax payments were calculated, the net profit was found, as shown in equation 6.4;

$$\text{Net Profit} = \sum_{n=1}^{10}(GP - D_n - T_n) = \sum_{n=1}^{10}(\text{Net Profit})_n \qquad (6.4)$$

The net profit was then used to calculate the cashflow for each year which equation 6.5 illustrates.

$$C_n = D_n + (\text{Net Profit})_n \qquad (6.5)$$

The last step in finding IRR was using the goalseek function in excel, setting equation 6.1 equal to zero by changing i, where the new value of i finally represents the IRR. Table 6.1 states the different IRRs for the six cases.

Table 6.1: The table gives calculated internal rate of return for all six cases.

Case	IRR [%]
Standard	18.92
Hydrogen - nitrogen ratio	18.83
Steam-carbon ratio	19.21
Front-end pressure	17.58
Mole fraction oxygen by membrane	19.57
Mole fraction oxygen by electrolysis	16.91

7   Discussion

7.1   Aspen HYSYS model

The feedstock were assumed to be pure methane, which is the main component in natural gas. It is known that the composition of natural gas varies depending on the location of extraction, so this was an approximation. If components like ethane and propane were to be taken into account the results would differ slightly. Methane is the hydrocarbon species with the highest hydrogen to carbon ratio and is assumed to be the absolute most ideal feedstock. The pressure and temperature of the methane entering the process is set to be 60 bar and 14°C respectively. This approximation was done to simulate that methane will be transported under pressure independently of method of transportation.

The reactors used in the HYSYS simulation is called gibbs reactors which calculated the thermodynamic equilibrium of the given reaction set. This can be done both with and without a temperature restriction. The primary reformer has a temperature set-point on the outlet at 731°C. This was done to match the ammonia plant, NII, Herøya. A closer inspection of the outlet composition reveals that the concentration of methane out of the reformer is very close to that of the real plant, even though NII uses a mixture of ethane and propane as feedstock. This might indicate that the outlet stream at NII is close to equilibrium and that the theoretical approximation is quite good.

Kinetics were not included in any of the reactors. This will definitely affect the results to some extent. Since the reason for using a catalyst is for selectivity and rate of reaction towards the thermodynamic equilibrium, the model will match NII quite well if the reactor outlets at NII are at equilibrium. The results for the reactor outlets in the standard case is a good fit with one exception: The synthesis reactor has a higher conversion than expected, which suggests that the synthesis reaction is slow, and therefore not at equilibrium in the outlet. Because of this the ammonia production in the HYSYS model might be higher than whats realistic.

A stoichiometric calculation of combusting hydrogen and methane were performed to calculate the outlet composition of the flue gas and thereby the ideal combustion product composition were found. This is the theoretical minimum mass flow at the given conditions and in a real situation an excess of air would be used. An excess of air will lead to an increase in the amount of methane needed for the combustion, but it will have a positive effect on the exergy balance. The flue gas is assumed to leave the primary reformer with a temperature of 760°C which is approximately the same as on NII. Further the flue gas is cooled down to 220°C thereby giving off energy which is calculated into the exergy balance. This is also similar to NII. The reason why the gas is not cooled down further is to prevent condensation of sulfuric acid in the outlet because a sulfur guard is normally not used on the gas burned in the reformer burners. In the simulation no sulfur is present, so the flue gas could have been cooled even further, but again, this approximation is done to get a realistic result.

The reaction sets in both the reformer and secondary reformer is found from the null spaces of the atom species matrix. By not including eventual biproducts in the atom

species matrix, there will not be any formation of such. With no catalysts implemented in the model, their characteristics such as selectivity and rate improvement is not included in the reactor. This makes it necessary to exclude biproducts, as the production rate of such would be unreasonable. When the conditions and compositions out of these reactors are investigated it seems like this is a good approximation.

The air compressor was assumed to be purely adiabatic without cooling between the compressor stages. This was a simplification done to avoid heating the air after the compressor before it enters the secondary reformer. This will influence the energy consumption as well as the cost of the compressor, but the process results will remain unaffected by this assumption. The pressure ratio over the different stages of the compressor was assumed to be constant. This assumption was done for the synthesis gas compressor as well. A constant pressure ratio will give a minimum energy consumption for a given number of compressor stages.

There is no temperature restriction on the secondary reformer. This was to promote the consumption of methane. All methane leaving the secondary reformer will act as an inert throughout the rest of the process, and is therefore considered a loss of potential hydrogen.

With regards to the two shift reactors, the reaction set is put to just the water-gas shift reaction. This implies that a known biproduct, methanol, is neglected. Even by doing so, the composition out of the last shift reactor seems very reasonable compared to NII. An explanation for this is that in a real situation, the outlet is not at equilibrium which is probably due to the catalyst being very selective towards the water gas shift reaction, and much less towards the production of methanol. The shift reactors operates without any fixed outlet temperatures thereby allowing the reaction to proceed to its full extent. The argument for this is similar to that of the secondary reformer. All carbon monoxide leaving the last shift reactor will be used to produce methane. This is considered a production loss. The conversion is done to prevent poisoning of the synthesis catalyst.

For removal of carbon dioxide four absorption towers are used with water as the absorbant. The water is assumed to be completely pure with a temperature of 5°C. The temperature assumption is quite reasonable in a northern country, but a more realistic solution is that the water is recycled after a desorbtion. This will imply that there is some carbon dioxide already in the water, but this is neglected. The mole fraction out of the absorption towers are fixed to a value corresponding to 0.3%, but it could be pushed to approach zero if enough water was used. A percentage of 0.3% is used to get realistic results. Using an amine-water mixture is more common, but a three phase absorbtion simulation was found to be difficult and very extensive.

In the methanation reactor the defined reaction set is the methanation of both carbon monoxide and carbon dioxide. There are no temperature limitations on the outlet of this reactor, allowing the reaction to proceed to its full extent. In the results of the simulations there were no carbon oxides leaving the reactor, which is the objective of the methanation reactor. This suggests that the reaction set can be argued.

When the gas enters the synthesis loop it is mixed with synthesis gas already in the

loop. Then it enters a preheater before the ammonia reactor. This heat exchanger is to simulate the preheating which conventionally happens on the shell-side of the ammonia reactor. This is a small modification which has zero to none effect on the simulation results. The ammonia reactor only has the ammonia reaction as a defined reaction set. In addition the outlet temperature was fixed to 300°C. This gives a very high conversion, so the simulated outlet composition of ammonia is above 50%. This is believed to be quite high, so here the model deviates significantly from NII. A high conversion gives a high production of ammonia. In addition it will reduce the shaft work and might have an affect on the purge.

In an actual ammonia factory the flash gas is commonly absorbed in water to retrieve the ammonia. This part of the process is totally excluded from the model. Instead, the flash gas is added to the recycle stream. A problem with possibly taking this flash gas out of the process would be that the inert concentration in the synthesis loop would be too low. The HYSYS model seems to have a too large interaction constant between methane and ammonia, leading to a higher amount of methane being absorbed in the liquid ammonia than would be expected. By totally excluding the part of the plant which retrieves ammonia from the flash gas as well as the purge gas, the operation and installation cost will be somewhat higher than the economic calculations suggest.

There is a purge to keep the sum of the inert concentrations at 10% into the reactor. The inert concentration into the reactor will effect the production. The optimal value was not investigated in this report. The ammonia in the purge gas was assumed to be possible to retrieve so it is added to the production, while methane and hydrogen is combusted in the primary reformer. By just adding the ammonia from the purge directly to the production without any extra work is a questionable approximation. However it was decided that not doing it would result in a bigger error, since the work done to retrieve the ammonia is quite small compared to the winnings of doing so.

7.2   HYSYS cases

In general for the different case studies there will be a margin of error due to the fact that kinetics is not accounted for. The kinetics is highly dependent on the partial pressures of the components, but this affect will not be seen in the HYSYS model used. Also another general case is that the pressure drops over the different components in the model is assumed constant. This is in reality not the case because the pressure drop is dependent on both volumetric flow rate and pressure, so the effect from this will not be seen.

When the oxygen cases was simulated the extra oxygen needed was supplied using a pure oxygen stream. This will be a good approximation when using electrolysis, but will not be realizable for the membrane separation. In the membrane case the oxygen enriched air produced will probably contain a maximum of 50% oxygen. In addition the hydrogen produced from electrolysis were assumed to be completely pure which makes it possible to add to the synthesis gas entering the compressor. Hydrogen from electrolysis is known to have a very high purity, so this assumption should be fine.

A summary of the results from the different cases is found in table 4.14. All results will

be discussed relative to the standard case. An overall result for all the cases were that the the amount of hydrogen into the synthesis gas compressor was increased relative to the standard case. Since the hydrogen to nitrogen ratio into the ammonia synthesis was set to 3, except for the hydrogen-nitrogen case, the amount of air compressed increased, increasing the shaft work. This also explains that all the cases has a relative increase in the shaft work.

7.2.1   Front-end pressure

In the optimized front-end pressure case it can be seen an increase in the total shaft work. This can be explained by that the pressure before the synthesis gas compressor was reduced with approximately 10 bar resulting in an increase in the shaft work done by the compressor. There was also a decrease in the shaft work done by the air compressor because the outlet pressure in the secondary reformer was reduced. A significant decrease in molar flow of methane could be seen out of the secondary reformer which was a result of the effect the decrease in pressure has on the equilibrium. This gave a higher hydrogen production which further on gave an increase in ammonia produced. This case has the highest operating profit relative to the standard case. The main variables from the case study are represented in table 4.4. A clear trend of increasing profit can be seen with decreasing inlet pressure until 50 bar. At this point the increase in ammonia produced was not large enough to compensate for the extra shaft work. This is also illustrated in figure 4.1.

7.2.2   Hydrogen-nitrogen ratio

The optimized hydrogen-nitrogen case had an increase in shaft work because of the most profitable hydrogen-nitrogen ratio was found to be 2.6. This means more air had to be added to the process, thereby leading to additional shaft work. The amount of methane leaving the secondary reformer was reduced which can be explained by the effect additional oxygen, being a reactant, has on the equilibrium. This gave slightly more hydrogen into the synthesis, but not as much as would be expected. This may indicate that some of the additional oxygen in the secondary reformer reacts with hydrogen to produce water and/or a reduced efficiency in the water-gas shift reaction. The additional nitrogen in the synthesis loop pushes the equilibrium towards the product side which lead to an increased ammonia production. The relative profit is quite high considering that this is the case with the smallest increase in hydrogen production. Important results from the case study is represented in table 4.6. Here it can be seen that an increase in the ratio was not profitable, but the relative operating profit increased with a decrease in the ratio down to 2.6. After this point the concentration of nitrogen in the synthesis loop was too high and the concentration of hydrogen was too low causing the ammonia production to drop whilst the shaft work kept on increasing. This created a clear maximum in the operating profit which can be seen in figure 4.2.

7.2.3   Steam-carbon ratio

Considering the optimized steam-carbon case a small increase in the shaft work could be seen, which most likely is due to the effect described above with the ratio being 3, and an increase in the hydrogen amount into the synthesis gas compressor. The amount of methane out of the secondary reformer was reduced as a result of an increased conversion of methane in the primary reformer which gave a decrease in methane entering the secondary reformer. The increase in steam will also promote the water gas shift, reaction giving a better conversion of carbon monoxide, thereby creating more hydrogen. The increase in hydrogen entering the synthesis loop resulted in an increase in the ammonia production. The ammonia production was almost as high as for the front end pressure case and the shaft work was considerably lower, but the profit is only the second largest. The explanation for this was that the price of the additional steam is taken into account. The trends from the case analysis can be seen in table 4.8. A decrease in the steam-carbon ratio gave a decrease in the profit relative to the standard case. This was caused by the decrease in the methane conversion in the primary reformer and water gas shift reaction. When the ratio was increased, the profit also increased until it reached 4.6. After this point the extra conversion of methane and carbon monoxide did not give enough increase in the ammonia production to compensate for the additional steam and shaft work. This trend can be seen in figure 4.3.

7.2.4   Mole fraction oxygen by membrane

The relative shaft work in the membrane case was the lowest of all the cases. Due to the fact that there were only a small extra amount of pure oxygen which needed to be compressed. The decrease in methane out of the secondary reformer is due to oxygen being a reactant, therefore pushing the equilibrium towards the product side. The hydrogen production was slightly increased giving a higher ammonia production. The relative operating profit for this case was the second smallest. Results from the case study can be seen in table 4.10. The profit increased until 0.235, after this point additional oxygen had a negative effect on the ammonia production. This can be explained by adding extra oxygen after this point will affect the water equilibrium in the secondary reformer, leading to a reduction in the hydrogen out of the reactor. Since most of the water was removed before the synthesis gas compressor the number of moles into this compressor will decrease. This explains the decrease in shaft work after the optimum was reached. This trend is illustrated in figure 4.4.

7.2.5   Mole fraction oxygen by electrolysis

In the electrolysis case the shaft work was also increased. The main contribution to this was the extra compressors needed to compress the hydrogen, which was put into the process before the synthesis gas compressor. The methane out of the secondary reformer was reduced for the same reason as for the membrane case. The increase in the hydrogen into the synthesis loop increased the ammonia production substantially. The reason for

the relative operating profit being the smallest of all the cases was that the electrolysis process demands large amount of energy, giving additional electricity expenses. Results from the case analysis can be seen in table 4.12. The trends is the same for the membrane case, but in contrast the shaft work kept on increasing after the optimum was reached. This was due to the increased hydrogen amount compressed in the additional compressor, which is independent of the number of moles entering the synthesis gas compressor. The optimum can also be seen in figure 4.5.

7.3   Discussing the profitability

Cost estimations are based on the total capital costs, variable costs, fixed costs, income and expenses. These are used to discuss the profitability analysis and to justify the results.

7.3.1   Total capital costs

Considering the cost of the compressors, it is known that the electrolysis case have more compressors than the other cases. The costs of the compressors in the electrolysis case are more expensive, whilst the others are more similar.

Looking at the costs of the reactors, R-2 to R-6, it seems reasonable that the front-end pressure case has the highest purchased costs. This is due to higher volumetric flow into the reactors. The primary reformer have the same costs for standard, hydrogen-nitrogen and mole fraction of oxygen by membrane and electrolysis case. This is because they have the same volumetric flow. The front-end pressure case and the steam-carbon case both have higher volumetric flow, so they will have a higher cost. This is because the cost of the standard case is used as a basis for the other cases.

Calculating the costs of the heat exchangers, a lot of assumptions were made. When calculating Δ T, it was assumed that the heating and cooling fluid was high pressure steam with the same temperature in and out of the exchanger. Theoretically, this might not be a good assumption, but using it to approximate the area, A, of the heat exchanger gives reasonable results. The hydrogen-nitrogen ratio and the steam-carbon case seem to differ significantly from the standard case. Areas calculated for heat exchangers H-20 and H-21 in hydrogen-nitrogen ratio case, are much higher than that of the standard case because of higher duty, Q. This is because of the excess of nitrogen in the synthesis loop. In the steam-carbon case, exchanger H-10 has a higher duty, because of condensation of extra steam, which affects the cost.

The costs estimations of the separators shows that the hydrogen-nitrogen ratio case is the most expensive. This is due to the fact that the volumetric flow rate of vapour is much higher in hydrogen-nitrogen ratio case than the standard case. The steam-carbon has a similar cost as the standard case. The other cases have a lower cost, mainly because of a smaller vapour flow into the synthesis separator.

All the absosrbers, except the absosrbers in the front-end pressure case, are similar. This is because the design pressures were set to the same. The pressure over the absosrbers in the front-end pressure case was 13.7 bar but in the other cases it was 23.7 bar. Therefore, the costs of the absosrbers in the front-pressure case are smaller than the other. A lower pressure demands a thinner shell of the absorbers.

The estimated purchased costs of the pumps are almost similar for all the cases. The front-end pressure case stand out from the others. The fact that the liquid flow into the pumps in the front-end pressure case are almost two times the flow of the other cases. The larger flow is a consequence of a reduced absorption efficiency at lower pressures. This leads to higher costs for the pumps.

In total, the calculated fixed costs in the cases seems reasonable. The standard case has the cheapest fixed costs, but the income and other expenses must be taken into account when considering the profitability. The front-end pressure case and the electrolysis case have the most expensive fixed capital costs. This might be because the compressors in the electrolysis case are expensive. Also, the front-end pressure case was slightly more expensive than the others. The reason might be the higher costs of the reactors, but also the costs of the compressor is high.

7.3.2 Variable costs of production

Variable costs of production are directly dependent on the operating rate and output. The cost of steam is the same for all cases except steam-carbon ratio. The assumption that the steam was medium pressure, MP, may cause some inaccuracy in the cost estimated. The steam in the HYSYS model is 30 bar and 300°C which means that in reality the cost of steam would be a little higher than estimated.

The cost of electricity for the compressors are pretty similar for all the cases except for the front-end pressure case. This makes sense because the pressure was 10 bar lower into the process compared to the other cases meaning the total shaft work increased for the front-end pressure case.

The cost of methane in the feed is constant for all cases. The cost of extra methane on the other hand is dependent on the amount of methane and hydrogen in the purge and the duty of R-1. The duty in the standard, hydrogen-nitrogen, electrolysis and membrane case is exactly the same, appendix B.2. The front-end pressure has the second highest duty and the steam-carbon case the highest. Since the amount of extra methane needed to heat R-1 had to fulfill the energy requirement. It makes sense that the steam-carbon has the highest cost for extra methane and front-pressure the second highest. For both of the cases, the reaction proceeded further than that of the standard case. In addition, the steam-carbon case, requires more energy to heat up the extra steam. The standard case has the lowest cost which seems reasonable because it has the highest amount of methane and hydrogen in the purge. It also seems reasonable that the hydrogen-nitrogen case is the third most expensive because of its low purge of hydrogen and methane. The same logic can be used when comparing the last two cases, membrane and electrolysis.

The membrane has a lower amount of hydrogen in its purge than electrolysis, therefore it should cost more.

The cost of extra oxygen in the membrane and electrolysis case are not comparable in terms of molar oxygen flows because the technology being used is different, and has different energy demands. The electrolysis only has oxygen as a biproduct and hydrogen as the main product. Meanwhile, oxygen is the main product in the membrane separation. Because of this, a higher cost per kmol pure oxygen can be justified for electrolysis as the additional hydrogen is of value.

The variable cost depends on cost of steam, compressor cost, cost of methane and cost of oxygen. The case with the highest variable costs is the steam-carbon case. This is because it has the highest cost of steam and the highest cost of methane. The second highest cost is the front-end pressure case because of its high compressor and methane costs. The third highest cost is the electrolysis case which is because of the high cost of oxygen. The third lowest cost is the hydrogen-nitrogen case which is higher than the other two because of its costs of methane and shaft work. The second lowest cost is the membrane case which is higher than the standard case mainly because of the extra oxygen and methane.

7.3.3   Fixed costs of production

Fixed costs of production is independent of the operating rate and output. It would not vary that much because only maintenance and property taxes were conducted from the ISBL. As seen from discussion about the total investment costs, the total fixed costs are highest for the electrolysis and the front-end pressure case. The standard case has the cheapest fixed costs due to the fact that the ISBL is the lowest.

7.3.4   Income

The income is proportional to the production output. The highest amount of ammonia produced is for the front-end pressure case, which is reasonable because more hydrogen goes into the synthesis. This achieves the highest income from ammonia. The exergy balance, which was an approximation of the energy balance for a heat integration, gave reasonable results. For all the cases the income from exergy was about 35 % of the cost of methane and steam, which is the main energy sources. The fact that the exergy balance gave a positive value, was expected, as a traditional ammonia plant has energy surplus. From table 5.18, the steam-carbon case has a higher income from exergy. The explanation for this is that more energy was introduced to the system by a higher amount of steam. By subtracting the additional cost of purchased steam, the income from exergy was actually quite like. So, there are small variations in the energy efficiency for the heat exchanging between the different cases.

7.3.5   Expenses

The annual operating expenses consisting of variable and fixed costs of production were lowest for the standard case. The membrane case was also one of the cases with the lowest expenses. From table 5.19 and table 5.20 it is important to notice that the income for all the cases are a lot higher than the expenses. This is a very important result for having a profitable project.

7.3.6   Profitability analysis

The gross profits, GP, are positive for all the cases. The calculated IRR are all higher than 15%. The higher IRR, the better investment.

The electrolysis case has the lowest IRR at 16.91%. The IRR is also lower than that of the standard case. This result is based on the assumptions made, but it seems reasonable because the production of oxygen through electrolysis is expensive. In addition the purchased cost of equipment is the most expensive, mostly because of the three extra compressors. This production method might be a of the future, but only if better technology provides cheaper possibilities.

The fifth best profitability was the front-end pressure case, with an IRR of 17.58%. This is lower than the standard case. It can be justified that also this alternative is a good investment due to the fact that the IRR is over 15%. This project has the advantage that it has the second best income, but the downsides are the high investment costs and the operating expenses.

The IRR for the hydrogen-nitrogen ratio case is 18.83%. This is just below the standard at 18.92%. This project places fourth considering the profitability. The gross profit, GP, is the second best of the cases, but it also has the fourth most expensive investment costs.

Calculated internal rate of return for standard case is the third highest. Even if the gross profit is the worst for this case, it has the lowest investment costs. This project has the lowest income because it produces the lowest amount of ammonia.

Two project seems to be better than the standard case. The steam-carbon ratio case has higher IRR than that of the standard. This case receives the highest GP result, even if the expenses are the highest of all the cases. One of the reason might be the fact that it has the best income result as shown in table 5.19. The income from both exergy analysis and the ammonia production are one of the best. The total investment costs are the third cheapest of the six cases.

The most profitable ammonia plant seem to be the production of ammonia by the case named mole fraction oxygen by membrane technology. The estimated IRR is 19.57%. This case will provide the most money. The reason for this internal rate is due to the second lowest investment costs for the plant. The fact that the fixed cost for the membrane was not included, means that the investment costs should be a little higher than estimated. It does not have the best income, but expenses are low. The low expenses were mainly based on low costs of the compressors, the steam, extra oxygen and the methane

feed. These costs are the second cheapest, only behind the standard case. The cost of the extra oxygen will remain the same as long as the oxygen price does not change. So, the most important thing to notice is that the membrane case does not have as many expenses, and provides more income than the standard case.

8   Conclusion and recommendations

This study indicates that two of the cases were more profitability than the standard case. These were the steam-carbon and the membrane case. This conclusion comes from the fact that the IRR = 19.21% and 19.57% respectively. In comparison to IRR of 18.92%, for the standard case, this implies that the modifications in these cases would improve the profit of the plant. The high IRR for the steam carbon case is mainly due to a high gross profit, while for the membrane it is the low extra expenses compared to the extra ammonia produced.

A suggestion for further investigation is to combine different cases with the objective of finding an absolute optimum. It may also be suggested to investigate the affect of changing the inert concentration. Before doing so it will be beneficial to include kinetics, especially in the synthesis reactor, to improve the model. The most interesting result from this study was the increased production with an increased oxygen mole fraction in the air-inlet. Because of this a proposal would be to further investigate this.

List of symbols

Make an alphabetic list of symbols used in the report with units and description. Latin and Greek symbols are listed in separate groups.

Table 8.1: Symbol list of the latin symbols used in this report

Symbol	Unit	Description
a	various	Cost constant
A	m^2	Area
b	various	Cost constant
c$_{p,\mathrm{avg}}$	J/K mol	Average heat capacity at constant pressure
C$_e$	US$	Purchased equipment cost
C$_{e,i}$	US$	Purchased equipment cost for unit i
C$_{e,i,SS}$	US$	Purchased equipment cost for unit i in stainless steel
C$_{e,i,NI}$	US$	Purchased equipment cost for unit i in nickel and inconel
C$_{\mathrm{NH_3}}$	NOK/kg	Price of ammonia
C$_{\mathrm{FC}}$	NOK	Total fixed capital cost
C$_{\mathrm{SS}}$	NOK	Total fixed capital cost for stainless steel
C$_{\mathrm{NI}}$	NOK	Total fixed capital cost for nickel and inconel
D	m	Absorber diameter
D$_v$	m	Vessel diameter
D&E	-	Estimation factor for Design and Engineering
e	kWh/kmol	Molar energy
E	kWh/h	Energy
f_j	-	Estimation factor of type j
f_c	-	Civil factor
f_{er}	-	Equipment erection factor
f_{el}	-	Electrial factor
f_i	-	Intrumentation and control factor
f_l	-	Lagging and paint factor
f_m	-	Material factor
f_p	-	Piping factor
f_s	-	Structures and buildings factor
Δ_fh	kWh/kmol	Molar enthalpy of formation
h$_{\mathrm{tot}}$	m	Total height of separator
h$_L$	m	Liquid level in separator
I$_i$	-	CEPCI index for year i
i	-	Interest rate
I$_{i,j}$	-	Ratio between CEPCI index for two years i,j
n	-	Exponent for type of equipment
$\hat{n}_i$	kmol/h	Molar flow of component i
$\hat{n}_{j,i}$	kmol/h	Molar flow of component i in stream j
m	kg	Absorber mass
$\hat{m}$	kg/s	mass flow of steam
$\hat{m}_i$	kg/h	Mass flow of component i

Symbol	Unit	Description
m_{shell}	kg	Shell mass in separators
$\hat{m}_i^*$	kg/h	Mass flow of component i in standard case
n_i	mole/s	Molar flow
OS	-	Estimation factor for offsites
P	kW	Effect
p_j	bar	Pressure in stream j
q	L/s	Liquid flow
Q	kW	Heat flow
S	various	Size parameter for equipments
T	K	Temperature
T_H	K	Temperature hot side
T_0	K	Temperature of the surroundings
T_{AM}	K	Mean arithmetic temperature
T_{LM}	K	Mean log temperature
t_w	m	Wall thickness
U	W/m^2 K	Overall heat transfer coefficient
u_s	m/s	Droplets settling velocity
u_t	m/s	Settling velocity
V	m^3	Volume
$\hat{V}_i$	m^3/s	Volumetric flow
V_v	m^3/s	vapour volumetric flow
W	kW	Shaft work done by compressors
W*	kW	Shaft work in the standard case
x_i	-	Mole fraction of component i
X	-	Estimation factor for contingency

Table 8.2: Symbol list of the greek symbols used in this report.

Symbol	Unit	Description
η	-	Effiency
η_{carnot}	-	Carnot effiency
π	-	Mathematical constant
ρ	kg/m^3	Density
ρ_L	kg/m^3	Density of liquid
ρ_V	kg/m^3	Density of vapour
τ	s	Residence time
ϕ	-	Void fraction

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A Conditions and mole fractions

A.1 Front-end pressure

A.1.1 Stream conditions

The most important conditions in and out of the main units in the front-end pressure case is presented in table A.1.

Table A.1: Conditions in and out of the units in the ammonia plant model calculated by HYSYS with optimized inlet pressure. p_{in} = 50 bar, x_{O_2} = 0.21, Steam/Carbon = 3.5, H_2/N_2 = 3 and $p_{synthesis}$ = 235 bar.

Stream	Vapor fraction [-]	Temperature [$°C$]	Presssure [bar]	Molar flow [kmol/h]
Inlet	1.0000	14	50.0	1247
Steam	1.0000	330	2049	4363
R1 in	1.0000	521	17.2	5610
R1 out	1.0000	730	16.7	7160
Air	1.0000	15	1.0	1764
Comp. Air	1.0000	506	16.7	1764
Oxygen	-	-	-	-
R2 in	1.0000	692	16.7	8924
R2 out	1.0000	927	16.6	9470
R3 in	1.0000	338	15.7	9470
R3 out	1.0000	409	14.8	9470
R4 in	1.0000	203	14.3	9470
R4 out	1.0000	219	14.0	9470
V1 in	0.7233	36	13.9	9470
V1 top	1.0000	36	13.9	6850
C1 in	1.0000	36	23.6	6850
C1 out	1.0000	6	13.4	5602
R5 in	1.0000	314	12.8	5602
R5 out	1.0000	347	12.6	5545
V2 in	0.9924	14	12.3	5545
V2 top	1.0000	14	12.3	5502
Hydrogen	-	-	-	-
V3 in	0.9994	15	25.7	5502
V3 top	1.0000	15	25.7	5499
V4 in	0.9997	15	53.8	5499
V4 top	1.0000	15	53.8	5497
V5 in	0.9999	15	112.4	5497
V5 top	1.0000	15	112.4	5497
V6 in	0.9999	15	235	5497
V6 top	1.0000	15	235	5496
R6 in	1.0000	200	235	8025
R6 out	1.0000	300	235	5362
V7 in	0.4457	5	225	5362
V7 top	1.0000	5	225	2390
V7 btm	0.0000	5	225	2972
V8 in	0.1106	-8	5	2972
V8 top	1.0000	-8	5	329
Ammonia	0.0000	-8	5	2644
Purge	1.0000	74	225	190
Recycle	1.0000	79	235	2528

A.1.2   Mole fractions

The mole fractions of the components in and out of the main units in the front-end pressure case is presented in table A.2.

Table A.2: Mole fractions in and out of the units in the ammonia plant model calculated by HYSYS with optimized inlet pressure. p_{in} = 50 bar, x_{O_2} = 0.21, Steam/Carbon = 3.5, H_2/N_2 = 3 and $p_{synthesis}$ = 235 bar.

Stream	x_{CH_4}	x_{H_2O}	x_{CO_2}	x_{CO}	x_{H_2}	x_{N_2}	x_{Ar}	x_{O_2}	x_{NH_3}
Inlet	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Steam	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
R1 in	0.2222	0.7778	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
R1 out	0.0659	0.4349	0.0663	0.0419	0.3910	0.0000	0.0000	0.0000	0.0000
Air in	0.0000	0.0000	0.0000	0.0000	0.0000	0.7800	0.0100	0.2100	0.0000
Comp. Air	0.0000	0.0000	0.0000	0.0000	0.0000	0.7800	0.0100	0.2100	0.0000
Oxygen	-	-	-	-	-	-	-	-	-
R2 in	0.0529	0.3489	0.0532	0.0336	0.3137	0.1542	0.0020	0.0415	0.0000
R2 out	0.0014	0.3553	0.0535	0.0767	0.3659	0.1453	0.0019	0.0000	0.0000
R3 in	0.0014	0.3553	0.0535	0.0767	0.3659	0.1453	0.0019	0.0000	0.0000
R3 out	0.0014	0.2930	0.1158	0.0144	0.4282	0.1453	0.0019	0.0000	0.0000
R4 in	0.0014	0.2930	0.1158	0.0144	0.4282	0.1453	0.0019	0.0000	0.0000
R4 out	0.0014	0.2798	0.1290	0.0012	0.4414	0.1453	0.0019	0.0000	0.0000
V1 in	0.0014	0.2798	0.1290	0.0012	0.4414	0.1453	0.0019	0.0000	0.0000
V1 out	0.0020	0.0046	0.1780	0.0017	0.6102	0.2009	0.0026	0.0000	0.0000
C in	0.0020	0.0046	0.1780	0.0017	0.6102	0.2009	0.0026	0.0000	0.0000
C out	0.0024	0.0007	0.0030	0.0021	0.7460	0.2426	0.0032	0.0000	0.0000
R5 in	0.0024	0.0007	0.0030	0.0021	0.7460	0.2426	0.0032	0.0000	0.0000
R5 out	0.0076	0.0089	0.0000	0.0000	0.7352	0.2451	0.0032	0.0000	0.0000
V2 in	0.0076	0.0089	0.0000	0.0000	0.7352	0.2451	0.0032	0.0000	0.0000
V2 out	0.0077	0.0013	0.0000	0.0000	0.7409	0.2470	0.0032	0.0000	0.0000
Hydrogen	-	-	-	-	-	-	-	-	-
V3 in	0.0077	0.0013	0.0000	0.0000	0.7409	0.2470	0.0032	0.0000	0.0000
V3 out	0.0077	0.0007	0.0000	0.0000	0.7413	0.2471	0.0032	0.0000	0.0000
V4 in	0.0077	0.0007	0.0000	0.0000	0.7413	0.2471	0.0032	0.0000	0.0000
V4 out	0.0077	0.0004	0.0000	0.0000	0.7415	0.2471	0.0032	0.0000	0.0000
V5 in	0.0077	0.0004	0.0000	0.0000	0.7415	0.2471	0.0032	0.0000	0.0000
V5 out	0.0077	0.0003	0.0000	0.0000	0.7417	0.2472	0.0032	0.0000	0.0000
V6 in	0.0077	0.0003	0.0000	0.0000	0.7417	0.2472	0.0032	0.0000	0.0000
V6 out	0.0077	0.0002	0.0000	0.0000	0.7417	0.2472	0.0032	0.0000	0.0000
R6 in	0.0687	0.0001	0.0000	0.0000	0.6456	0.2152	0.0313	0.0000	0.0390
R6 out	0.1028	0.0002	0.0000	0.0000	0.2215	0.0738	0.0469	0.0000	0.5549
V7 in	0.1028	0.0002	0.0000	0.0000	0.2215	0.0738	0.0469	0.0000	0.5549
V7 top	0.1920	0.0000	0.0000	0.0000	0.4901	0.1624	0.1016	0.0000	0.0539
V7 btm	0.0310	0.0004	0.0000	0.0000	0.0055	0.0026	0.0029	0.0000	0.9577
V8 in	0.0310	0.0004	0.0000	0.0000	0.0055	0.0026	0.0029	0.0000	0.9577
V8 top	0.2691	0.0000	0.0000	0.0000	0.0495	0.0231	0.0257	0.0000	0.6326
Ammonia	0.0014	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9981
Purge	0.2013	0.0000	0.0000	0.0000	0.4368	0.1456	0.0924	0.0000	0.1238
Recycle	0.2013	0.0000	0.0000	0.0000	0.4368	0.1456	0.0924	0.0000	0.1238

A.2 Hydrogen-Nitrogen case

A.2.1 Stream conditions

The most important conditions in and out of the main units in the hydrogen-nitrogen ratio case is presented in table A.3.

Table A.3: Conditions in and out of the units in the ammonia plant model calculated by HYSYS with optimized N2/H2 ratio. $p_{in} = 60$ bar, $x_{O_2} = 0.21$, Steam/Carbon = 3.5, $H_2/N_2 = 2.6$ and $p_{synthesis} = 235$ bar.

Stream	Vapor fraction [-]	Temperature [°C]	Pressure [bar]	Mole flow [kmol/h]
Inlet	1.0000	14	60.0	1247
Steam	1.0000	330	30.4	4363
R1 in	1.0000	521	27.2	5610
R1 out	1.0000	732	26.7	6943
Air in	1.0000	15	1.0	1978
Comp. Air	1.0000	634	26.6	1978
Oxygen	-	-	-	-
R2 in	1.0000	713	26.6	8921
R2 out	1.0000	945	26.5	9624
R3 in	1.0000	338	25.6	9624
R3 out	1.0000	407	24.7	9624
R4 in	1.0000	203	24.2	9624
R4 out	1.0000	217	23.9	9624
V1 in	0.7156	36	23.8	9624
V1 out	1.0000	36	23.6	6887
C in	1.0000	36	23.6	6887
C out	1.0000	6	23.2	5655
R5 in	1.0000	314	22.6	5655
R5 out	1.0000	346	22.5	5599
V2 in	0.9923	14	22.2	5599
V2 out	1.0000	14	22.2	5556
Hydrogen	-	-	-	-
V3 in	0.9997	15	39.9	5556
V3 out	1.0000	15	39.9	5554
V4 in	0.9998	15	72.1	5554
V4 out	1.0000	15	72.1	5554
V5 in	0.9999	15	130.2	5554
V5 out	1.0000	15	130.2	5553
V6 in	~1.0000	15	235	5553
V6 out	1.0000	15	235	5553
R6 in	1.0000	200	235	11725
R6 out	1.0000	300	235	9119
V7 in	0.6895	5	225	9119
V7 top	1.0000	5	225	6287
V7 btm	0.0000	5	225	2832
V8 in	0.0897	-6	5	2832
V8 top	1.0000	-6	5	254
Ammonia	0.0000	-6	500	2578
Purge	1.0000	26	225	369
Recycle	1.0000	31	235	6172

A.2.2   Mole fractions

The mole fractions of the components in and out of the main units in the hydrogen-nitrogen ratio case is presented in table A.4.

Table A.4: Mole fractions in and out of the units in the ammonia plant model calculated by HYSYS with optimized H2/N2 ratio. p_{in} = 60 bar, x_{O_2} = 0.21, Steam/Carbon = 3.5, H_2/N_2 = 2.6 and $p_{synthesis}$ = 235 bar.

Stream	x_{CH_4}	x_{H_2O}	x_{CO_2}	x_{CO}	x_{H_2}	x_{N_2}	x_{Ar}	x_{O_2}	x_{NH_3}
Inlet	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Steam	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
R1 in	0.2222	0.7778	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
R1 out	0.0836	0.4697	0.0627	0.0333	0.3507	0.0000	0.0000	0.0000	0.0000
Air in	0.0000	0.0000	0.0000	0.0000	0.0000	0.7800	0.0100	0.2100	0.0000
Comp. Air	0.0000	0.0000	0.0000	0.0000	0.0000	0.7800	0.0100	0.2100	0.0000
Oxygen	-	-	-	-	-	-	-	-	-
R2 in	0.0650	0.3656	0.0488	0.0259	0.3507	0.1730	0.0022	0.0466	0.0000
R2 out	0.0022	0.3597	0.0526	0.0747	0.3484	0.1603	0.0021	0.0000	0.0000
R3 in	0.0022	0.3597	0.0526	0.0747	0.3484	0.1603	0.0021	0.0000	0.0000
R3 out	0.0022	0.2982	0.1141	0.0132	0.4098	0.1603	0.0021	0.0000	0.0000
R4 in	0.0022	0.2982	0.1141	0.0132	0.4098	0.1603	0.0021	0.0000	0.0000
R4 out	0.0022	0.2861	0.1262	0.0011	0.4220	0.1603	0.0021	0.0000	0.0000
V1 in	0.0022	0.2861	0.1262	0.0011	0.4220	0.1603	0.0021	0.0000	0.0000
V1 out	0.0030	0.0029	0.1759	0.0016	0.5897	0.2240	0.0029	0.0000	0.0000
C in	0.0030	0.0029	0.1759	0.0016	0.5897	0.2240	0.0029	0.0000	0.0000
C out	0.0037	0.0005	0.0030	0.0019	0.7181	0.2694	0.0035	0.0000	0.0000
R5 in	0.0037	0.0005	0.0030	0.0019	0.7181	0.2694	0.0035	0.0000	0.0000
R5 out	0.0087	0.0085	0.0000	0.0000	0.7073	0.2720	0.0035	0.0000	0.0000
V2 in	0.0087	0.0085	0.0000	0.0000	0.7073	0.2720	0.0035	0.0000	0.0000
V2 out	0.0088	0.0008	0.0000	0.0000	0.7127	0.2741	0.0036	0.0000	0.0000
Hydrogen	-	-	-	-	-	-	-	-	-
V3 in	0.0088	0.0008	0.0000	0.0000	0.7127	0.2741	0.0036	0.0000	0.0000
V3 out	0.0088	0.0005	0.0000	0.0000	0.7129	0.2742	0.0036	0.0000	0.0000
V4 in	0.0088	0.0005	0.0000	0.0000	0.7129	0.2742	0.0036	0.0000	0.0000
V4 out	0.0088	0.0003	0.0000	0.0000	0.7131	0.2743	0.0036	0.0000	0.0000
V5 in	0.0088	0.0003	0.0000	0.0000	0.7131	0.2743	0.0036	0.0000	0.0000
V5 out	0.0088	0.0003	0.0000	0.0000	0.7131	0.2743	0.0036	0.0000	0.0000
V6 in	0.0088	0.0003	0.0000	0.0000	0.7131	0.2742	0.0036	0.0000	0.0000
V6 out	0.0088	0.0002	0.0000	0.0000	0.7132	0.2743	0.0036	0.0000	0.0000
R6 in	0.0701	0.0001	0.0000	0.0000	0.4102	0.4434	0.0299	0.0000	0.0462
R6 out	0.0902	0.0001	0.0000	0.0000	0.0988	0.4273	0.0384	0.0000	0.3452
V7 in	0.0902	0.0001	0.0000	0.0000	0.0988	0.4273	0.0384	0.0000	0.3452
V7 top	0.1230	0.0000	0.0000	0.0000	0.1425	0.6158	0.0550	0.0000	0.0636
V7 btm	0.0172	0.0004	0.0000	0.0000	0.0016	0.0088	0.0014	0.0000	0.9705
V8 in	0.0172	0.0004	0.0000	0.0000	0.0017	0.0088	0.0014	0.0000	0.9705
V8 top	0.1822	0.0000	0.0000	0.0000	0.0184	0.0983	0.0153	0.0000	0.6858
Ammonia	0.0010	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9985
Purge	0.1253	0.0000	0.0000	0.0000	0.1377	0.5957	0.0535	0.0000	0.0878
Recycle	0.1253	0.0000	0.0000	0.0000	0.1377	0.5957	0.0535	0.0000	0.0878

A.3   Steam/carbon ratio case

A.3.1   Stream conditions

The most important conditions in and out of the main units in the steam-carbon ratio case is presented in table A.5.

Table A.5: Conditions in and out of the units in the ammonia plant model calculated by HYSYS with optimized steam/carbon ratio. $p_{in} = 60$ bar, $x_{O_2} = 0.21$, Steam/Carbon = 4.6, $H_2/N_2 = 3$ and $p_{synthesis} = 235$ bar.

Stream	Vapor fraction [-]	Temperature [$°C$]	Presssure [bar]	Molar flow [kmol/h]
Inlet	1.0000	14	60.0	1247
Steam	1.0000	330	30.4	5735
R1 in	1.0000	521	27.2	6981
R1 out	1.0000	730	26.7	8513
Air	1.0000	15	1.0	1761
Comp. Air	1.0000	634	26.6	1761
Oxygen	-	-	-	-
R2 in	1.0000	716	26.6	10274
R2 out	1.0000	917	26.5	10823
R3 in	1.0000	338	25.6	10823
R3 out	1.0000	392.8	24.7	10823
R4 in	1.0000	203	24.2	10823
R4 out	1.0000	211	23.9	10823
V1 in	0.6290	33	23.8	10823
V1 top	1.0000	36	23.6	6808
C1 in	1.0000	36	23.6	6808
C1 out	1.0000	6	23.3	5576
R5 in	1.0000	314	22.6	5576
R5 out	1.0000	341	22.5	5528
V2 in	0.9929	14	22.2	5528
V2 top	1.0000	14	22.2	5489
Hydrogen	-	-	-	-
V3 in	0.9997	15	39.9	5489
V3 top	1.0000	15	39.9	5488
V4 in	0.9998	15	72.1	5488
V4 top	1.0000	15	72.1	5487
V5 in	0.9999	15	130.2	5487
V5 top	1.0000	15	130.2	5486
V6 in	~1.0000	15	235	5486
V6 top	1.0000	15	235	5486
R6 in	1.0000	200	235	7996
R6 out	1.0000	300	235	5343
V7 in	0.4452	5	225	5343
V7 top	1.0000	5	225	2379
V7 btm	0.0000	5	225	2964
V8 in	0.1116	-8	5	2964
V8 top	1.0000	-8	5	331
Ammonia	0.0000	-8	5	2633
Purge	1.0000	74	225	199
Recycle	1.0000	79	235	2510

A.3.2   Mole fractions

The mole fractions of the components in and out of the main units in the steam-carbon ratio case is presented in table A.6.

Table A.6: Mole fractions in and out of the units in the ammonia plant model calculated by HYSYS with optimized steam/carbon ratio. p_{in} = 60 bar, x_{O_2} = 0.21, Steam/Carbon = 4.6, H_2/N_2 = 3 and $p_{synthesis}$ = 235 bar.

Stream	x_{CH_4}	x_{H_2O}	x_{CO_2}	x_{CO}	x_{H_2}	x_{N_2}	x_{Ar}	x_{O_2}	x_{NH_3}
Inlet	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Steam	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
R1 in	0.1786	0.8214	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
R1 out	0.0564	0.5215	0.0621	0.0279	0.3321	0.0000	0.0000	0.0000	0.0000
Air	0.0000	0.0000	0.0000	0.0000	0.0000	0.7800	0.0100	0.2100	0.0000
Comp. Air	0.0000	0.0000	0.0000	0.0000	0.0000	0.7800	0.0100	0.2100	0.0000
Oxygen	-	-	-	-	-	-	-	-	-
R2 in	0.0468	0.4321	0.0515	0.0231	0.2752	0.1337	0.0017	0.0360	0.0000
R2 out	0.0019	0.4293	0.0556	0.0576	0.3270	0.1269	0.0016	0.0000	0.0000
R3 in	0.0019	0.4293	0.0556	0.0576	0.3270	0.1269	0.0016	0.0000	0.0000
R3 out	0.0019	0.3794	0.1055	0.0077	0.3769	0.1269	0.0016	0.0000	0.0000
R4 in	0.0019	0.3794	0.1055	0.0077	0.3769	0.1269	0.0016	0.0000	0.0000
R4 out	0.0019	0.3723	0.1126	0.0006	0.3840	0.1269	0.0016	0.0000	0.0000
V1 in	0.0019	0.3723	0.1126	0.0006	0.3840	0.1269	0.0016	0.0000	0.0000
V1 top	0.0031	0.0029	0.1783	0.0010	0.6105	0.2017	0.0026	0.0000	0.0000
C1 in	0.0031	0.0029	0.1783	0.0010	0.6105	0.2017	0.0026	0.0000	0.0000
C1 out	0.0038	0.0005	0.0031	0.0012	0.7452	0.2431	0.0032	0.0000	0.0000
R5 in	0.0038	0.0005	0.0031	0.0012	0.7452	0.2431	0.0032	0.0000	0.0000
R5 out	0.0081	0.0079	0.0000	0.0000	0.7356	0.2452	0.0032	0.0000	0.0000
V2 in	0.0081	0.0079	0.0000	0.0000	0.7356	0.2452	0.0032	0.0000	0.0000
V2 top	0.0082	0.0008	0.0000	0.0000	0.7409	0.2470	0.0032	0.0000	0.0000
Hydrogen	-	-	-	-	-	-	-	-	-
V3 in	0.0082	0.0008	0.0000	0.0000	0.7409	0.2470	0.0032	0.0000	0.0000
V3 top	0.0082	0.0005	0.0000	0.0000	0.7411	0.2470	0.0032	0.0000	0.0000
V4 in	0.0082	0.0005	0.0000	0.0000	0.7411	0.2470	0.0032	0.0000	0.0000
V4 top	0.0082	0.0003	0.0000	0.0000	0.7412	0.2471	0.0032	0.0000	0.0000
V5 in	0.0082	0.0003	0.0000	0.0000	0.7412	0.2471	0.0032	0.0000	0.0000
V5 top	0.0082	0.0002	0.0000	0.0000	0.7413	0.2471	0.0032	0.0000	0.0000
V6 in	0.0082	0.0002	0.0000	0.0000	0.7413	0.2471	0.0032	0.0000	0.0000
V6 top	0.0082	0.0002	0.0000	0.0000	0.7413	0.2471	0.0032	0.0000	0.0000
R6 in	0.0702	0.0001	0.0000	0.0000	0.6456	0.2151	0.0230	0.0000	0.0391
R6 out	0.1051	0.0002	0.0000	0.0000	0.2214	0.0738	0.0446	0.0000	0.5550
V7 in	0.1051	0.0002	0.0000	0.0000	0.2214	0.0738	0.0446	0.0000	0.5550
V7 top	0.1964	0.0000	0.0000	0.0000	0.4903	0.1625	0.0967	0.0000	0.0541
V7 btm	0.0318	0.0004	0.0000	0.0000	0.0055	0.0026	0.0027	0.0000	0.9570
V8 in	0.0318	0.0004	0.0000	0.0000	0.0055	0.0026	0.0027	0.0000	0.9570
V8 top	0.2733	0.0000	0.0000	0.0000	0.0493	0.0230	0.0244	0.0000	0.6300
Ammonia	0.0014	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9981
Purge	0.2058	0.0000	0.0000	0.0000	0.4365	0.1454	0.0879	0.0000	0.1244
Recycle	0.2058	0.0000	0.0000	0.0000	0.4365	0.1454	0.0879	0.0000	0.1244

A.4   Mole fraction oxygen by membrane separation of air

A.4.1   Stream conditions

The most important conditions in and out of the main units in the mole fraction oxygen by membrane case is presented in table A.7.

Table A.7: Conditions in and out of the units in the ammonia plant model calculated by HYSYS with optimized mole fraction O_2, x_{O_2}, in the air inlet by addition of pure O_2 using membrane separation of air. $p_{in} = 60$ bar, $x_{O_2} = 0.235$, Steam/Carbon = 3.5, $H_2/N_2 = 3$ and $p_{synthesis} = 235$ bar.

Stream	Vapor fraction [-]	Temperature [$^\circ C$]	Presssure [bar]	Molar flow [kmol/h]
Inlet	1.0000	14	60.0	1247
Steam	1.0000	330	30.4	4363
R1 in	1.0000	521	27.2	5610
R1 out	1.0000	732	26.7	6943
Air	1.0000	15	1.0	1717
Comp. Air	1.0000	633	26.6	1773
Oxygen	1.0000	15	1.0	56
R2 in	1.0000	715	26.6	8716
R2 out	1.0000	951	26.5	9420
R3 in	1.0000	338	25.6	9420
R3 out	1.0000	408	24.7	9420
R4 in	1.0000	203	24.2	9420
R4 out	1.0000	217	23.9	9420
V1 in	0.7094	36	23.8	9420
V1 top	1.0000	36	23.6	6682
C1 in	1.0000	36	23.6	6682
C1 out	1.0000	6	23.3	5451
R5 in	1.0000	314	22.6	5451
R5 out	1.0000	347	22.5	5397
V2 in	0.9923	14	22.2	5397
V2 top	1.0000	14	22.2	5355
Hydrogen	-	-	-	-
V3 in	0.9997	15	39.9	5355
V3 top	1.0000	15	39.9	5354
V4 in	0.9998	15	72.1	5354
V4 top	1.0000	15	72.1	5353
V5 in	0.9999	15	130.2	5353
V5 top	1.0000	15	130.2	5353
V6 in	~1.0000	15	235	5353
V6 top	1.0000	15	235	5353
R6 in	1.0000	200	235	7791
R6 out	1.0000	300	235	5207
V7 in	0.4452	5	225	5207
V7 top	1.0000	5	225	2318
V7 btm	0.0000	5	225	2889
V8 in	0.1125	-9	5	2889
V8 top	1.0000	-9	5	325
Ammonia	0.0000	-9	5	2564
Purge	1.0000	74	225	204
Recycle	1.0000	79	235	2439

A.4.2   Mole fractions

The mole fractions of the components in and out of the main units in the mole fraction oxygen by membrane case is presented in table A.6.

Table A.8: Mole fractions in and out of the units in the ammonia plant model calculated by HYSYS with optimized mole fraction O_2, x_{O_2}, in the air inlet by addition of pure O_2 using membrane separation of air. p_{in} = 60 bar, x_{O_2} = 0.235, Steam/Carbon = 3.5, H_2/N_2 = 3 and $p_{synthesis}$ = 235 bar.

Stream	x_{CH_4}	x_{H_2O}	x_{CO_2}	x_{CO}	x_{H_2}	x_{N_2}	x_{Ar}	x_{O_2}	x_{NH_3}
Inlet	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Steam	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
R1 in	0.2222	0.7778	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
R1 out	0.0836	0.4697	0.0627	0.0333	0.3507	0.0000	0.0000	0.0000	0.0000
Air	0.0000	0.0000	0.0000	0.0000	0.0000	0.7800	0.0100	0.2100	0.0000
Comp. Air	0.0000	0.0000	0.0000	0.0000	0.0000	0.7553	0.0097	0.0235	0.0000
Oxygen	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
R2 in	0.0666	0.3742	0.0500	0.0265	0.2794	0.1536	0.0020	0.0478	0.0000
R2 out	0.0021	0.3680	0.0534	0.0769	0.3557	0.1422	0.0018	0.0000	0.0000
R3 in	0.0021	0.3680	0.0534	0.0769	0.3557	0.1422	0.0018	0.0000	0.0000
R3 out	0.0021	0.3049	0.1165	0.0137	0.4188	0.1422	0.0018	0.0000	0.0000
R4 in	0.0021	0.3049	0.1165	0.0137	0.4188	0.1422	0.0018	0.0000	0.0000
R4 out	0.0021	0.2923	0.1291	0.0012	0.4314	0.1422	0.0018	0.0000	0.0000
V1 in	0.0021	0.2923	0.1291	0.0012	0.4314	0.1422	0.0018	0.0000	0.0000
V1 top	0.0029	0.0029	0.1815	0.0016	0.6081	0.2004	0.0026	0.0000	0.0000
C1 in	0.0029	0.0029	0.1815	0.0016	0.6081	0.2004	0.0026	0.0000	0.0000
C1 out	0.0036	0.0005	0.0030	0.0020	0.7453	0.2425	0.0031	0.0000	0.0000
R5 in	0.0036	0.0005	0.0030	0.0020	0.7453	0.2425	0.0031	0.0000	0.0000
R5 out	0.0087	0.0085	0.0000	0.0000	0.7348	0.2449	0.0032	0.0000	0.0000
V2 in	0.0087	0.0085	0.0000	0.0000	0.7348	0.2449	0.0032	0.0000	0.0000
V2 top	0.0087	0.0008	0.0000	0.0000	0.7405	0.2468	0.0032	0.0000	0.0000
Hydrogen	-	-	-	-	-	-	-	-	-
V3 in	0.0087	0.0008	0.0000	0.0000	0.7405	0.2468	0.0032	0.0000	0.0000
V3 top	0.0087	0.0005	0.0000	0.0000	0.7407	0.2469	0.0032	0.0000	0.0000
V4 in	0.0087	0.0005	0.0000	0.0000	0.7407	0.2469	0.0032	0.0000	0.0000
V4 top	0.0087	0.0003	0.0000	0.0000	0.7408	0.2469	0.0032	0.0000	0.0000
V5 in	0.0087	0.0003	0.0000	0.0000	0.7408	0.2469	0.0032	0.0000	0.0000
V5 top	0.0087	0.0002	0.0000	0.0000	0.7409	0.2469	0.0032	0.0000	0.0000
V6 in	0.0087	0.0002	0.0000	0.0000	0.7409	0.2469	0.0032	0.0000	0.0000
V6 top	0.0087	0.0002	0.0000	0.0000	0.7409	0.2470	0.0032	0.0000	0.0000
R6 in	0.0716	0.0001	0.0000	0.0000	0.6456	0.2152	0.0284	0.0000	0.0391
R6 out	0.1072	0.0002	0.0000	0.0000	0.2215	0.0738	0.0425	0.0000	0.5548
V7 in	0.1072	0.0002	0.0000	0.0000	0.2215	0.0738	0.0425	0.0000	0.5548
V7 top	0.2002	0.0000	0.0000	0.0000	0.4908	0.1626	0.0922	0.0000	0.0543
V7 btm	0.0325	0.0004	0.0000	0.0000	0.0055	0.0026	0.0027	0.0000	0.9564
V8 in	0.0325	0.0004	0.0000	0.0000	0.0055	0.0026	0.0027	0.0000	0.9564
V8 top	0.2770	0.0000	0.0000	0.0000	0.0491	0.0230	0.0231	0.0000	0.6278
Ammonia	0.0015	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9981
Purge	0.2097	0.0000	0.0000	0.0000	0.4364	0.1454	0.0837	0.0000	0.1248
Recycle	0.2097	0.0000	0.0000	0.0000	0.4364	0.1454	0.0837	0.0000	0.1248

A.5   Mole fraction oxygen by electrolysis of water

A.5.1   Stream conditions

The most important conditions in and out of the main units in the mole fraction oxygen by electrolysis case is presented in table A.9.

Table A.9: Conditions in and out of the units in the ammonia plant model calculated by HYSYS with optimized mole fraction O_2, x_{O_2}, in the air inlet by addition of pure O_2 from electrolysis. $p_{in} = 60$ bar, $x_{O_2} = 0.231$, Steam/Carbon = 3.5, $H_2/N_2 = 3$ and $p_{synthesis} = 235$ bar.

Stream	Vapor fraction [-]	Temperature [$°C$]	Presssure [bar]	Molar flow [kmol/h]
Inlet	1.0000	14	60.0	1247
Steam	1.0000	330	30.4	4363
R1 in	1.0000	521	27.2	5610
R1 out	1.0000	732	26.7	6943
Air	1.0000	15	1.0	1758
Comp. Air	1.0000	633	26.6	1806
Oxygen	1.0000	15	1.0	48
R2 in	1.0000	715	26.6	8748
R2 out	1.0000	951	26.5	9452
R3 in	1.0000	338	25.6	9452
R3 out	1.0000	408	24.7	9452
R4 in	1.0000	203	24.2	9452
R4 out	1.0000	218	23.9	9452
V1 in	0.7103	36	23.8	9452
V1 top	1.0000	36	23.6	6714
C1 in	1.0000	36	23.6	6714
C1 out	1.0000	6	23.3	5483
R5 in	1.0000	314	22.6	5483
R5 out	1.0000	347	22.5	5428
V2 in	0.9922	14	22.2	5428
V2 top	1.0000	14	22.2	5385
Hydrogen	1.0000	14	1.0	96
V3 in	0.9997	15	39.9	5482
V3 top	1.0000	15	39.9	5480
V4 in	0.9998	15	72.1	5480
V4 top	1.0000	15	72.1	5479
V5 in	0.9999	15	130.2	5479
V5 top	1.0000	15	130.2	5479
V6 in	~1.0000	15	235	5479
V6 top	1.0000	15	235	5479
R6 in	1.0000	200	235	7979
R6 out	1.0000	300	235	5332
V7 in	0.4454	5	225	5332
V7 top	1.0000	5	225	2375
V7 btm	0.0000	5	225	2957
V8 in	0.1123	-8	5	2957
V8 top	1.0000	-8	5	332
Ammonia	0.0000	-8	5	2625
Purge	1.0000	74	225	207
Recycle	1.0000	79	235	2450

A.5.2   Mole fractions

The mole fractions of the components in and out of the main units in the mole fraction oxygen by electrolysis case is presented in table A.6.

Table A.10: Mole fractions in and out of the units in the ammonia plant model calculated by HYSYS with optimized mole fraction O_2, x_{O_2}, in the air inlet by addition of pure O_2 from electrolysis. $p_{in} = 60$ bar, $x_{O_2} = 0.231$, Steam/Carbon $= 3.5$, $H_2/N_2 = 3$ and $p_{synthesis} = 235$ bar.

Stream	x_{CH_4}	x_{H_2O}	x_{CO_2}	x_{CO}	x_{H_2}	x_{N_2}	x_{Ar}	x_{O_2}	x_{NH_3}
Inlet	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Steam	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
R1 in	0.2222	0.7778	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
R1 out	0.0836	0.4697	0.0627	0.0333	0.3507	0.0000	0.0000	0.0000	0.0000
Air	0.0000	0.0000	0.0000	0.0000	0.0000	0.7800	0.0100	0.2100	0.0000
Comp. Air	0.0000	0.0000	0.0000	0.0000	0.0000	0.7593	0.0097	0.2310	0.0000
Oxygen	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
R2 in	0.0663	0.3728	0.0498	0.0264	0.2783	0.1567	0.0020	0.0477	0.0000
R2 out	0.0021	0.3668	0.0532	0.0766	0.3544	0.1450	0.0019	0.0000	0.0000
R3 in	0.0021	0.3668	0.0532	0.0766	0.3544	0.1450	0.0019	0.0000	0.0000
R3 out	0.0021	0.3039	0.1161	0.0137	0.4173	0.1450	0.0019	0.0000	0.0000
R4 in	0.0021	0.3039	0.1161	0.0137	0.4173	0.1450	0.0019	0.0000	0.0000
R4 out	0.0021	0.2914	0.1287	0.0011	0.4296	0.1450	0.0019	0.0000	0.0000
V1 in	0.0021	0.2914	0.1287	0.0011	0.4296	0.1450	0.0019	0.0000	0.0000
V1 top	0.0029	0.0029	0.1806	0.0016	0.6052	0.2042	0.0026	0.0000	0.0000
C1 in	0.0029	0.0029	0.1806	0.0016	0.6052	0.2042	0.0026	0.0000	0.0000
C1 out	0.0036	0.0005	0.0030	0.0020	0.7410	0.2468	0.0032	0.0000	0.0000
R5 in	0.0036	0.0005	0.0030	0.0020	0.7410	0.2468	0.0032	0.0000	0.0000
R5 out	0.0087	0.0086	0.0000	0.0000	0.7302	0.2493	0.0032	0.0000	0.0000
V2 in	0.0087	0.0086	0.0000	0.0000	0.7302	0.2493	0.0032	0.0000	0.0000
V2 top	0.0087	0.0008	0.0000	0.0000	0.7360	0.2513	0.0033	0.0000	0.0000
Hydrogen	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000
V3 in	0.0086	0.0008	0.0000	0.0000	0.7406	0.2467	0.0032	0.0000	0.0000
V3 top	0.0086	0.0005	0.0000	0.0000	0.7408	0.2469	0.0032	0.0000	0.0000
V4 in	0.0086	0.0005	0.0000	0.0000	0.7408	0.2469	0.0032	0.0000	0.0000
V4 top	0.0086	0.0003	0.0000	0.0000	0.7409	0.2470	0.0032	0.0000	0.0000
V5 in	0.0086	0.0003	0.0000	0.0000	0.7409	0.2470	0.0032	0.0000	0.0000
V5 top	0.0086	0.0002	0.0000	0.0000	0.7410	0.2470	0.0032	0.0000	0.0000
V6 in	0.0086	0.0002	0.0000	0.0000	0.7410	0.2470	0.0032	0.0000	0.0000
V6 top	0.0086	0.0002	0.0000	0.0000	0.7410	0.2470	0.0032	0.0000	0.0000
R6 in	0.0712	0.0001	0.0000	0.0000	0.6456	0.2151	0.0288	0.0000	0.0391
R6 out	0.1066	0.0002	0.0000	0.0000	0.2216	0.0739	0.0430	0.0000	0.5547
V7 in	0.1066	0.0002	0.0000	0.0000	0.2216	0.0739	0.0430	0.0000	0.5547
V7 top	0.1992	0.0000	0.0000	0.0000	0.4907	0.1626	0.0933	0.0000	0.0542
V7 btm	0.0323	0.0004	0.0000	0.0000	0.0055	0.0026	0.0026	0.0000	0.9567
V8 in	0.0323	0.0004	0.0000	0.0000	0.0055	0.0026	0.0026	0.0000	0.9567
V8 top	0.2760	0.0000	0.0000	0.0000	0.0491	0.0230	0.0234	0.0000	0.6284
Ammonia	0.0015	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.9981
Purge	0.2086	0.0000	0.0000	0.0000	0.4365	0.1455	0.0847	0.0000	0.1247
Recycle	0.2086	0.0000	0.0000	0.0000	0.4365	0.1455	0.0847	0.0000	0.1247

B   Economic calculations

B.1   Primary reformer

The primary reformer was calculated using values and information from a book about catalytic steam reforming and information received from the ammonia plant in Porsgrunn, Norway[20]. The first assumption made was that since the material price of the metal probably generates the biggest cost for the reformer, the metal volume of the tubes should be calculated. The length of the tubes was assumed to be 10 m. According to the fore-mentioned book the values for length of reformer tubes usually varies between 6-12 m. The assumed value of 10 m gave ratio to estimate the diameter, thickness and number of tubes.

$$\Delta l = 10 - 6 = 4 \tag{B.1}$$

$$\Delta l_{100\%} = 12 - 6 = 6 \tag{B.2}$$

$$x = \frac{\Delta l}{\Delta l_{100\%}} = \frac{4}{6} \tag{B.3}$$

The internal diameter was said to vary between 0.07-0.16 m. Using the factor x along with the given data from the book to obtain

$$\Delta d = x \Delta d_{100\%} \tag{B.4}$$

where $\Delta d_{100\%}$ is the maximum value for d, $0.16m - 0.07m = 0.09m$. This gives the diameter for one tube:

$$d = d_{min} + \Delta d \tag{B.5}$$

where d_{min} is the minimum value for d, 0.07m. This type of scaling from assumed height to diameter was done the same way for number of tubes, N, and wall thickness, t_w, which gives the volume of metal in the tubes, $V_{TotMetal}$. The volume of a cylinder including wall thickness was first calculated. Then the inner volume of a cylinder was substracted from the outer volume which was assumed to be the metal volume of one tube in the reformer. The total volume of metal was calculated from multiplying the volume of metal in one tube with number of tubes. The variation of tubes was said in the fore-mentioned book to be between 40-400, and the wall thickness between 0.01-0.02m. Equation A.6-A.9 shows how the volumes were calculated and the calculated values are shown in table B.1.

$$V_{outer} = \pi \left(\frac{d + 2t_w}{2} \right)^2 l \tag{B.6}$$

$$V_{\text{inner}} = \pi \left(\frac{\text{d}}{2}\right)^2 \text{l} \tag{B.7}$$

$$V_{\text{metal}} = V_{\text{outer}} - v_{\text{inner}} \tag{B.8}$$

$$V_{\text{TotMetal}} = V_{\text{metal}} N \tag{B.9}$$

Table B.1: The table is showing the calculated size values for the primary reformer

Variable calculated	Values
l	10 m
d	0.17 m
t_w	0.02 m
V_{outer}	0.39 m^3
V_{inner}	0.25 m^3
V_{metal}	0.15 m^3
V_{TotMetal}	41.03 m^3
N	280

In the end the inlet volume flow of each case was divided by the inlet volume flow of the standard case where this ratio was multiplied by the volume in the bottom row of table B.1. The estimated costs for the different cases is illustrated in table 5.3

B.2   Heat exchangers

When the investment costs of the heaters and coolers in the HYSYS model were to be calculated, they were viewed at as heat exchangers. The assumption was made that the heating or cooling fluid was high pressure steam, therefore having a high heat capacity so it can be assumed to have the same temperature into the heat exchanger as out. Equation B.10 was rearranged in order to get the estimated area[m^2] of each heater and cooler which in the end gives the investment costs by using equation 5.7.

$$Q = UA\Delta T_{\text{AM}} \tag{B.10}$$

Where A is the area [m^2], Q [W] is the duty value collected from HYSYS, U [W/m^2 ^{o}C] the heat transfer coefficient, assumed 400 and ΔT [^{o}C] as shown in equation B.11. The assumption of the pressurized fluid with the same in and out temperature, where the temperature equals the out temperature of the actual process flow, justifies equation B.11.

$$\Delta T_{\text{AM}} = \frac{\Delta T1 - \Delta T2}{2} = \frac{T_{\text{out}} - T_{\text{in}}}{2} \tag{B.11}$$

ΔT_{AM} is the arithmetic mean temperature difference between inlet hot and cold and outlet hot and cold. Figure B.1 shows an example of how the approximation was made.
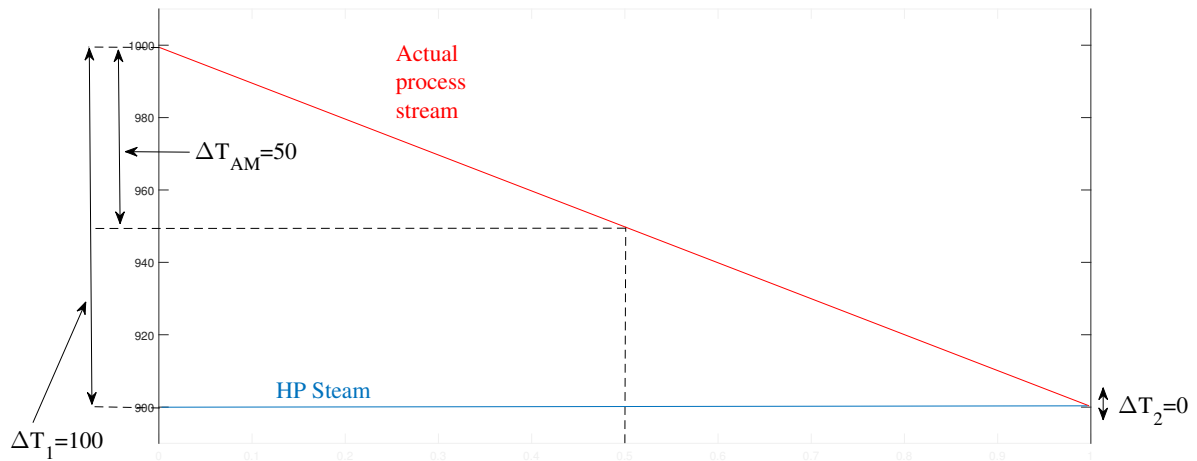

Figure B.1: Assumed temperature profile of heat exchangers. The cold side inlet is assumed to be equal in temperature to outlet hot side i.e $\Delta T_2 = 0$ whereas cold side outlet still has the same temperature but inlet hot side has a different value i.e $\Delta T_1 = 100$. According to the arithmetic mean temperature difference will then be 50.

B.3   Wall thickness, t_w

To calculate the wall thickness used in calculations for estimation of the purchased cost of the separators and the absorbers, equation B.12 was used.

$$t_w = \frac{p_{design} D_v}{(2SE) - (1.2P_{design})} \tag{B.12}$$

Where the design pressure, p_{design} [N/m^2], of the vessel is 10 % of the operating pressure [N/m^2], which is gathered from simulations. D_v [m] is the diameter of the vessel, SE is the shear stress for stainless steel 304 which is 89 N^2/mm^2.

B.4   Absorbers

The mass of the pressure vessels were calculated from the volume of the wall, bottom and top of a cylinder. Volume of the pressure vessel sylinder were calculated as in B.13

$$V_{syl} = \pi \frac{d_{syl}^2}{4} h_{syl} \tag{B.13}$$

where d_{syl} and h_{syl} is the diameter [m] and the height [m] of the vessel. The desired volume for calculating the mass of the pressure vessel, is equation B.14

$$V_{wall} = V_{syl} - \pi \frac{(d_{syl} - 2 * t_w)^2}{4} h_{syl} \tag{B.14}$$

where t_w is calculated from equation B.12. Volume of the top and bottom were calculated as equation B.15

$$V_{top+btm} = \pi \frac{d_{syl}^2}{4} t_w \cdot 2 \tag{B.15}$$

Total volume [m^3] of pressure vessel :

$$V_{tot} = V_{wall} + V_{top+btm} \tag{B.16}$$

Equation B.16 were used to find the mass [kg] of the pressure vessels in stainless steel 304 as in B.17:

$$m = V_{tot} * \rho_{ss304} \tag{B.17}$$

Here, ρ_{ss304} is the mass density [kg/m^3] of stainless steel 304. Mass, m, were used in calculating the cost of the pressure vessel in the separators in 5.14.

B.5   Separators

Volume of liquid held in the vessel was calculated as in equation B.18 for a minimum hold up of 10 minutes:

$$V_L = \hat{V}_L(10 \cdot 60) \tag{B.18}$$

Here $\hat{V}_L$, is the liquid volumetric flow [m³/s]. The liquid depth required is calculated from equation B.19:

$$h_L = \frac{V_L}{\pi \cdot \frac{D_v^2}{4}} \tag{B.19}$$

B.6   Exergy calculations

To estimate the exergy available at the plant, values from simulations in Aspen HYSYS were used. Temperatures in, T_{H1}, and out, T_{H2} of the heaters/coolers and R-1 were used to estimate the carnot efficiency. The carnot effieciency is defined as in equation B.20 [21]:

$$\eta_{carnot} = 1 - \frac{T_C}{T_{H,lm}} \tag{B.20}$$

where T_C is the cold tremprature outside, assumed do be 5 °C. $T_{H,lm}$ is the logaritmic mean temprature om hot side, given in B.21:

$$T_{H,lm} = \frac{T_{H2} - T_{H1}}{ln\frac{T_{H2}}{T_{H1}}} \tag{B.21}$$

The second law of thermodynamics states that the total entropy always increases as given in B.22 [21]:

$$\Delta S_{total} = \Delta S + \Delta S_{sur} \geq 0 \tag{B.22}$$

An ideal (reversible) process gives

$$\Delta S_{total} = 0 \tag{B.23}$$

which in addition to the first law of the thermodynamics can be used to estimate the ideal work. The temperature for the surroundings have constant temperature, T_0, so the entropy for the surroundings is given by

$$\Delta S_{sur} = \Delta S_0 = \frac{-Q}{T_0} \tag{B.24}$$

where Q is added heat from the surroundings to the process. Substituted into B.22 gives B.25

$$Q \leq T_0 \Delta S \tag{B.25}$$

When B.25 is substituted into the first law of thermodynamics, B.26 for a stationary continous process:

$$\Delta H = W_s + Q \tag{B.26}$$

the result is B.27

$$W_s \leq \Delta H - T_0 \Delta S \tag{B.27}$$

This shows that $W_s \leq W_s^{id}$. Then the ideal (reversible) work for the surroundings at constant temperature, T_0, is given in B.28:

$$W_s^{id} = \Delta H - T_0 \Delta S \tag{B.28}$$

W_s^{id} is the "minimal work needed to supply the system", which is equivalent to the fact that $-W_s^{id}$ is the "maximum work you can take out of the system".

Using B.28 to show that exergy, B, is defined as:

$$B \hat{=} E + pV - T_0 S \tag{B.29}$$

Assuming that only internal energy contributes to energy, E = U, and the exergy becomes B.30

$$B = H - T_0 S \tag{B.30}$$

For a stationary continous process we have B.31:

$$W_s^{id} = \Delta B = \Delta H - T_0 \Delta S \tag{B.31}$$

Here, change in the systems exergy, Δ B is equal to the available work that theoretically can be taken at a given change of state compared to surroundings at a constant temperature, T_0.

To calculate the exergy, duties [kJ/h] were taken from simulations in Aspen HYSYS and implemented as in equation B.32:

$$B = \text{Duty} \cdot \eta_{carnot} \tag{B.32}$$

B.7   Extra oxygen used in 3.1.4

To find the certain energy amount and cost of producing oxygen from membrane, values from Christer Haugaland in Air Products, were used as given in appendix C. The volumetric flow of air in to the membrane is $\hat{V}_1$=31 000 Nm^3/h. Out of the membrane, the volumetric flow is $\hat{V}_2$=15 000 Nm^3/h, with x$_{2,n_2}$=0.95. To get the desired amount of $\hat{V}_2$ with x_{2,n_2}=0,95 it requires an energy of 870 kJ/Nm^3(N$_2$) (P= 1 atm and T=0°). The volumetric flow [Nm^3/h] of air in the second outlet of the membrane, is given in B.33:

$$\hat{V}_3 = 31000 - 15000 = 16000 \text{Nm}^3/\text{h} \tag{B.33}$$

Amount of nitrogen dioxide in the second outlet was calculated from B.35:

$$\hat{V}_1 x_{1,n_2} = \hat{V}_2 x_{2,n_2} + \hat{V}_3 x_{3,n_2} \tag{B.34}$$

$$x_{3,n_2} = \frac{\hat{V}_1 x_{1,n_2} - \hat{V}_2 x_{2,n_2}}{\hat{V}_3} \tag{B.35}$$

$$x_{3,n_2} = \frac{0,79 \cdot 31000 - 0,95 \cdot 15000}{16000} = 0.64 \tag{B.36}$$

Assuming that air only consist of oxygen dioxide and nitrogen dioxide, amount of oxygen out of second exit is x_{3,O_2}=0,36. Volumetric flow of oxygen dioxide out at second exit is:

$$\hat{V}_{3,O2} = \hat{V}_3 x_{3,O_2} = 5760 \text{Nm}^3/\text{h} \tag{B.37}$$

$$\hat{n_{O_2}} = \frac{5760}{22.414} = 257 \text{kmole/h} \tag{B.38}$$

Energy amount of 870 kJ/Nm^3(N$_2$) were used to find the effect [kWh/h]:

$$P = 87015000 = 13.05 \text{GJ/h} = 3625 \text{kWh/h} \tag{B.39}$$

$$e_{O_2} = \frac{3625 \text{kWh/h}}{257 \text{kmol/h}} = 14.1 \text{kWh/kmol}(O_2) \tag{B.40}$$

Equation B.40 were used to find the price per kmole of oxygen. This gave 4.23 NOK/kmole(O_2). Then, 56 kmole/h into the secondary reformer costs 230 NOK/h.

B.8   Extra oxygen used in 3.1.5

The use of electrolysis as an additional supplier of hydrogen also gave rise to an extra oxygen cost. The value of 3.8 kWh/Nm^3(H_2) was used to calculate the extra oxygen cost[5]. Equation B.41 shows how this was done.

$$e_{O_2} = 3.8\frac{\text{kWh}}{\text{Nm}^3(H_2)} \cdot 22.414\frac{\text{Nm}^3(H_2)}{\text{kmol}(H_2)} \cdot 2\frac{\text{kmol}(H_2)}{\text{kmol}(O_2)} = 170.3464\frac{\text{kWh}}{\text{kmol}(O_2)} \tag{B.41}$$

The ratio 2 kmol(H_2)/kmol(O_2) was derived from equation 3.3. The next step was to use the molar flow of oxygen into the secondary reformer from the HYSYS model. The value 47.98 kmol(O_2)/h was found and with an electricity price of 0.3 NOK/kWh the extra cost of oxygen ended up at 2452 NOK/h.

B.9   Extra methane

The amount of extra methane needed to supply the primary reformer with sufficient thermal energy was calculated by setting up an energy balance. The duty in R-1, E_{R-1}, a value taken from the HYSYS model, was the amount of energy needed to heat up the reformer. The combustion energy of methane and hydrogen was set equal to the duty plus the energy needed to heat up the combustion products, or fluegas.

$$E_{\text{R-1}} + \hat{n}_{\text{tot,flue}}c_{\text{P,avg}}\Delta T = (\hat{n}_{\text{CH}_4,\text{P}} + \hat{n}_{\text{CH}_4,\text{extra}})\Delta_{\text{f}}h_{\text{CH}_4} + \hat{n}_{\text{H}_2,\text{P}}\Delta_{\text{f}}h_{\text{H}_2} \tag{B.42}$$

In equation B.42 E_{R-1} is the duty from R-1, $\hat{n}_{\text{tot,flue}}$ the total molar flow of the fluegas, $c_{\text{P,avg}}$ the average heat capacity of the fluegas, ΔT the assumed temperature difference for the combustion, $\hat{n}_{\text{CH}_4,\text{P}}$ the molar flow of methane from purge, $\hat{n}_{\text{CH}_4,\text{extra}}$ the extra molar flow of methane needed to heat the reformer, $\Delta_{\text{f}}h_{\text{CH}_4}$ the molar formation enthalpy for methane using SI values and equation B.43, $\hat{n}_{\text{H}_2,\text{P}}$ the molar of hydrogen from the purge and $\Delta_{\text{f}}h_{\text{H}_2}$ the molar formation enthalpy for hydrogen using SI values and equation B.44[26].

$$CH_4 + 2O_2 = CO_2 + 2H_2O \tag{B.43}$$

$$2H_2 + O_2 = 2H_2O \tag{B.44}$$

The fluegases was assumed to consists of nitrogen, argon, carbon dioxide and water. They were based on the stoichiometric relationship between oxygen and air, as well as the two equations B.43 and B.44. The air going into the combustion chamber was assumed to be

21% oxygen, 78% nitrogen and 1% argon. The equation set B.45 shows how the extra methane was included in the calculation of the combustion reactants and products.

$$
\begin{aligned}
\hat{n}_{O_2} &= 2\left(\hat{n}_{CH_4,extra} + \hat{n}_{CH_4,P}\right) + 0.5\hat{n}_{H_2,P} \\
\hat{n}_{air} &= \frac{\hat{n}_{O_2}}{0.21} \\
\hat{n}_{N_2,flue} &= 0.78\hat{n}_{air} \\
\hat{n}_{Ar,flue} &= 0.01\hat{n}_{air} \\
\hat{n}_{CO_2,flue} &= \hat{n}_{CH_4,P} + \hat{n}_{CH_4,extra} \\
\hat{n}_{H_2O,flue} &= 2\left(\hat{n}_{CH_4,P} + \hat{n}_{CH_4,extra}\right) + \hat{n}_{H_2,P} \\
\hat{n}_{tot,flue} &= \hat{n}_{N_2,flue} + \hat{n}_{Ar,flue} + \hat{n}_{CO_2,flue} + \hat{n}_{H_2O,flue}
\end{aligned}
\tag{B.45}
$$

The mole fraction of component i in the fluegas was then calculated from equation B.46

$$
x_i = \frac{\hat{n}_{i,flue}}{\hat{n}_{tot,flue}}
\tag{B.46}
$$

After this the c_P for the respective fluegas was found by taking the average c_P value from JANAF tables on the temperature interval 220-760°C[27]. Each average c_P value was then weighted against their respective mole fraction and summed up to the heat capacity $c_{P,avg}$ in equation B.42 was found. The duty and purge values from the HYSYS model is shown in table B.2.

Table B.2: The table shows the duty and purge values from HYSYS model for all six cases.

Case	E_{R-1} [kWh/h]	$\hat{n}_{CH_4,P}$ [kmol/h]	$\hat{n}_{H_2,P}$ [kmol/h]
Standard	53023	79	142
Hydrogen-nitrogen ratio	53023	46	51
Steam-arbon ratio	61494	41	87
Front-end pressure	59139	38	83
Mole fraction oxygen by membrane	53023	43	82
Mole fraction oxygen by electrolysis	53023	43	90

In the end when all the equations was inserted in excel, the "goalseek" function was used to make equation B.42 add up by changing the value of $\hat{n}_{CH_4,extra}$. This value was then converted into the desired unit, kg/h, before calculating the price of this extra methane. The extra amount is shown in table B.3.

B.10 Excel calculations - standard case

Exergy

Enhet	H-1	H-2	H-3	H-4	H-5
T_in	287,16	363,55	392,55	552,56	640,97
T_out	363,55	392,55	426,32	640,97	794,05
n_carnot	0,14	0,26	0,32	0,53	0,61
Duty[kJ/3600h=kW	-162,77	-123,30	-170,35	-3084,85	-6396,74
Electricty	-97,66	-73,98	-102,21	-1850,91	-3838,04
Price	-29,30	-22,19	-30,66	-555,27	-1151,41

H-6	H-7	H-8	H-9	H-10	H-11
1168,77	687,10	676,49	557,11	490,05	279,36
687,10	611,07	557,11	476,11	309,15	453,17
0,69	0,57	0,55	0,46	0,29	0,23
31228,75	3839,51	5819,88	3257,97	13872,34	-1729,84
18737,25	2303,71	3491,93	1954,78	8323,40	-1037,90
5621,17	691,11	1047,58	586,43	2497,02	-311,37

H-12	H-13	H-14	H-15	H-16	H-17
453,17	619,41	520,16	346,16	358,29	359,87
587,17	520,16	346,16	287,16	288,16	288,16
0,46	0,51	0,35	0,12	0,14	0,14
-2773,40	2270,26	2673,61	367,32	417,15	436,15
-1664,04	1362,16	1604,17	220,39	250,29	261,69
-499,21	408,65	481,25	66,12	75,09	78,51

H-18	H-19	H-20	H-21	R1	SUM
360,02	360,30	307,94	573,26	1033,00	
288,16	288,16	473,15	278,18	493,00	
0,14	0,14	0,28	0,32	0,62	
443,84	456,36	-3075,21	9514,49	10867,08	
266,31	273,82	-1845,13	5708,69	6520,25	
79,89	82,15	-553,54	1712,61	1956,07	12230,69

Compressors		K-1	K-2	K-3	K-4
centrifugal [kW]		1117,27	1423,20	1812,56	4719,57
a	490000,00				
b	16800,00				
n	0,60				
C_e		1622935,05	1799991,00	2004553,79	3179370,34
		K-5	K-6	K-7	K-8
		3096,37	3162,40	3244,92	3399,23

	K-5	K-6	K-7	K-8
2578436,39	2605042,80	2637985,86	2698704,31	

	K-9	K-13	SUM
	114,82	1633,53	

	779286,53	1912935,20	21819241,28

Cost [NOK 2(	256217269,81
Stainless ste.	1,30

Reactors		void fraction	R-2	R-3	R-4
tau [s]		0,45	5,00	5,00	5,00
V_flow [m^3/s]			7,29	5,13	4,21
V [m^3]			81,05	56,98	46,73
a	53000,00				
b	28000,00				
n	0,80				
			995231,89	763734,47	659488,71
			R-5	R-6	
			5,00	33,00	
			3,30	0,39	
			36,67	28,70	
			552545,64	463663,37	

C_e   3434664,09

Cost u/R1 [31024848,67

	R-1	SUM R1	SUM		
				delta(l)	4,00
V_outer	0,39			delta(l_100%)	6,00
V_inner	0,25			delta(l)/delta(l_1	0,67
V_wall	0,15			delta(d)	0,11
Tubes	280,00			delta(t_w)	0,01
d=delta(d)+d_min	0,18			delta(d_min)	0,07
t_w=delta(t_w)+t_	0,02			delta(t_w_min)	0,01
l	10,00			delta(N)	240,00
V_all_tubes	41,03	599554,66		delta(N_min)	40,00
fm(Ni Inconel)/fm(	1,31	7082062,45 [NOK 2016]			

Exchangers		H-1	H-2	H-3	H-4
U[W/m^2K]		400,00	400,00	400,00	400,00
Q[W]		1153540,69	467273,80	531959,33	5787356,36
DelT		38,20	14,50	16,89	44,21
Shell and tube A [m^2]		75,50	80,58	78,75	327,29
a	24000,00				
b	46,00		33,95		
n	1,20				
		32246,98	32917,83	32675,05	71938,06

H-5	H-6	H-7	H-8	H-9	H-10
400,00	400,00	400,00	400,00	400,00	400,00
10471945,16	-45048752,39	-6724578,87	-10627810,39	-7075510,54	-47567073,78
76,54	-240,83	-38,02	-59,69	-40,50	-90,45
342,05	467,64	442,19	445,12	436,78	1314,75
74544,33	97561,03	92784,78	93332,19	91776,13	278313,17

H-11	H-12	H-13	H-14	H-15	H-16
400,00	400,00	400,00	400,00	400,00	400,00
7661015,19	5999632,33	-4446457,86	-7661000,17	-3086098,15	-3066751,79
86,90	67,00	-49,62	-87,00	-29,50	-35,07
220,39	223,87	224,02	220,14	261,51	218,65
53826,07	54391,00	54415,52	53784,98	60621,66	53542,39

H-17	H-18	H-19	H-20	H-21	SUM
400,00	400,00	400,00	400,00	400,00	
-3160632,17	-3212035,35	-3294444,44	11107939,75	-29883261,69	
-35,86	-35,93	-36,07	82,61	-147,54	
220,37	223,48	228,34	336,18	506,36	
53821,48	54328,59	55120,68	73503,58	104930,09	1570375,60

C_e	1570375,60
Cost[NOK 2010	18440483,05
Stainless steal	1,30

Separators	V-1	V-2	V-3	V-4	V-5
rho_L [kg/m^3]	1000,00	1016,00	1016,00	1017,00	1018,00
rho_v [kg/m^3]	13,77	8,00	14,21	25,15	43,76
u_t [m/s]	0,59	0,79	0,59	0,44	0,33
Vv [m^3/s]	2,01	1,62	0,91	0,52	0,30
Dv [m]	2,08	1,62	1,41	1,22	1,07
Dv(ft round up)	6,81	5,32	4,62	4,01	3,51
NY Dv [m]	2,13	1,52	1,52	1,22	1,22
V_L [m^3/s]	0,01	0,00	0,00	0,00	0,00
Hold up time [s]	600,00	600,00	600,00	600,00	600,00
Volume held in ve	8,10	0,12	0,00	0,00	0,00
h_v	2,27	0,07	0,00	0,00	0,00
h_tot [m]	5,87	2,75	2,69	2,23	2,23
P_operating	2385000,00	2216000,00	7211000,00	7211000,00	13020000,00
P_design [N/m^2	2623500,00	2437600,00	7932100,00	7932100,00	14322000,00
SE (shear stress S	89000000,00	89000000,00	89000000,00	89000000,00	89000000,00
t_w (m)	0,03	0,02	0,07	0,06	0,11
rho (stainless stee	8030,00	8030,00	8030,00	8030,00	8030,00
Shellmass [kg]	10102,64	2245,26	7412,17	3937,09	7443,74
a	15000,00				
b	68,00				
n	0,85				
C_e [$ USGC 200	187297,30	62982,75	147422,76	92340,64	147901,90

Separators	V-6	V-7	V-8		
rho_L [kg/m^3]	1021,00	608,30	642,90		
rho_v [kg/m^3]	73,96	112,30	3,90		
u_t [m/s]	0,25	0,15	0,90		
Vv [m^3/s]	0,18	0,07	0,40		
Dv [m]	0,94	0,78	0,75		
Dv(ft round up)	3,10	2,55	2,48		
NY Dv [m]	0,91	0,91	0,61		
V_L [m^3/s]	0,00	0,02	0,02		
Hold up time [s]	600,00	600,00	600,00		
Volume held in ve	0,00	13,18	11,01		
h_v	0,00	20,08	37,75		
h_tot [m]	1,77	21,85	39,07		
P_operating	23500000,00	22500000,00	500000,00		
P_design [N/m^2	25850000,00	24750000,00	550000,00		
SE (shear stress S	89000000,00	89000000,00	89000000,00		
t_w (m)	0,16	0,15	0,00		
rho (stainless stee	8030,00	8030,00	8030,00		
Shellmass [kg]	6572,30	76894,31	1135,31		
a					
b					
n					
C_e [$ USGC 200	134555,28	982206,03	41875,41		
C_e [$ USGC 200	1796582,07				
Cost [NOK 2016]	16228278,90				

Absorber		C-1	C-2	C-3	C-4
sievetrays					
diameter [m]		1,50	1,50	1,50	1,50
a	110,00				
b	380,00				
n	1,80				
C_e [$ 2007]		898,40	898,40	898,40	898,40
P_design [N/m^2]		2601500,00	2601500,00	2601500,00	2601500,00
t_w		0,02	0,02	0,02	0,02
V_sylinder [m^3]		16,83	16,83	16,83	16,83
h_sylinder [m]		9,50	9,50	9,50	9,50
V_vegg[m^3]		1,04	1,04	1,04	1,04
V_ToppBunn [m^3]		0,08	0,08	0,08	0,08
V_tot_steel [m^3]		1,12	1,12	1,12	1,12
rho_stainlesssteal 8.03 g/cm^3 --> [kg		8030,00	8030,00	8030,00	8030,00
pressure vessel, vertical 304 ss [kg]		8960,30	8960,30	8960,30	8960,30
a	15000,00				
b	68,00				
n	0,85				
C_e [$2007]		170590,57	170590,57	170590,57	170590,57
SUM(sieve tr	3593,61				
SUM(Vessels	682362,28				
Cost [NOK 20	6196145,28				

PUMPS		P-1	P-2	P-3	P-4
single-stage sentrifugal, flow [L/s]		622,50	622,50	622,50	622,50
a	6900,00				
b	206,00				
n	0,90				
C_e [$]		74289,56	74289,56	74289,56	74289,56
Explosion proof motor, power [kW]		1717,00	1717,00	1717,00	1717,00
a	-950,00				
b	1770,00				
n	0,60				
C_e [$]		153516,90	153516,90	153516,90	153516,90
C_e_pump [NOK 2016]	10700271,46				

fm (ss)	1,30
f_m(Ni Inconel)	1,70
f_m(ss)	1,30
f_er	0,30
f_p	0,80
f_i	0,30
f_el	0,20
f_c	0,30
f_s	0,20
f_l	0,10
OS	0,30
D&E	0,30
X	0,10
C_ei_A [NOK 2016]	338807297,17
C u/R1 [NOK 2016]	974722531,86
C R1 [NOK 2016]	18579999,14
C [NOK 2016]	993302531,00 ISBL
Tot fixed cap cost	1807810606,43

C_cap(2016) [NOK]	**1807810606,43** fixed

Methane recycle costs		
Mol CH4 [mol/h]	78668,00	fra hysys
Mol H2 [mol/h]	142101,00	fra hysys
dHrx(H2) (kWh/mol H2)	-0,07	
dHrx(CH4) (kWh/mol CH4)	-0,22	
Duty R1 [kWh/h] heat energ	53023,46	fra hysys
n_CH4 [mol/h]	222979,43	222979,43
n_O2 [mol/h]	674345,36	beregnet mengde o2 som trengs
Mengde luft [mol/h]	3211168,38	
n_N2 [mol/h]	2504711,34	Røykgass består av N2,Ar,CO2,H20
n_Ar [mol/h]	32111,68	
n_CO2 [mol/h]	301647,43	
n_H20 [mol/h]	745395,86	
n_tot_fluegas [mol/h]	3583866,31	
x_N2	0,70	
x_Ar	0,01	
x_CO2	0,08	
x_H2O	0,21	
Cp_N2 [J/K*mol]	29,12	
Cp_Ar [J/K*mol]	20,79	
Cp_CO2 [J/K*mol]	49,47	
Cp_H20 [J/K*mol]	38,25	
Cp_avg [kWh/K*mol]	0,00	
E=nCPdT [kWh]	17556,84	duty fra fluegas
Electricty [kWh/h]	10534,10	
kg(CH4)/h excess	3567,67	

	0,00	0,00	Energy balance

Natural Gas Price (NOK / N	24,37	per 2016 sept	24,37
1 BTU	1,06	GJ	1,06
feed [kg/h]	20000,00		3567,67
dHrx_CH4 [kJ/kmol]	-804000,00		-804000,00
price natural gas [NOK/GJ]	23,10		23,10
Mm_CH4 [kg/kmol]	16,05		16,05
føde [kmol/h]	1245,95		222,26
feed [kJ/h]	1001744330,92		178694703,93
feed [GJ/h]	1001,74		178,69
Price CH4 [NOK/h]	23139,82		4127,76

Amount of Product NH3 [kg/	43200,00		
Cost Product[NOK/h]	96446,91	844874935,27	nOK/YEAR

Steam production cost calculation			Compressor costs	
Molar flow steam[kmol/h]		4363,00	total duty [kW] = [kW	30590,00
Molar mass H2O[kg/kmol]		18,00		77527296,00
Mass flow steam[ton/h]		78,53	Cost [NOK/h]	9177,00
Price MP steam[£/ton]		8,76		
NOK/£(13:37 15.11.2016)		10,46		
Price [NOK/h]		7195,92		
Fixed costs of production			Variable costs	
salary operators (15 op	7441891,24		cost CH4 [NOK/year]	230356534,89
supervision	1860472,81		cost of steam [NOK/y	60791139,63
direct salary overhead	4837229,30	40-60% av opera	compressor costs	291147674,52
eiendomsskatt	29779075,93	3-5%ISBL		
vedlikehold	9933025,31	1-2%ISBL fixed cap		
	53871694,59			
annual sale income [NOK/year]				
product [NOK/year]	814783499,22			
exergy [NOK/year]	103324834,7			
SUM	918108333,92			

Annual service expenses	Annual income
345019369,11	918108333,92

Working capital	Investment
90390530,32	1807810606,43

Regneark for beregning av nåverdi og/eller intern rente.

Verdier som må innsettes nedenfor er i fet kursiv. Velg avskrivningsprinsipp.

År --->	Grunnl.data	-1	0	1	2
Investement	**1807,810606**				
working capital	90,39053032				
2)Amount depreciation 20%	20				
Depreciation Factor ,amount depreciation				0,2	0,1600
Industrial investment			-1807,8106		
Working capital			-90,39053		
Recover of service capital					
Annual sale income	918,1083339			918,11	918,11
Annual service expenses	422,5466651			422,55	422,55
Brutto service result				495,56	495,56
Depreciation				361,56	289,25
Result before taxes				134,00	206,31
Tax,Percentaje 28%	28			37,52	57,77
Net profit				96,48	148,54
Despreciation				361,56	289,25
Net cash flow			-1807,81	458,04	437,79
Accumula Net cash flow		0	-1898,20	-1440,16	-1002,37
Discount factor at rentage	18,91718893		1	0,8409	0,7071
Discount NKS			-1807,8106	385,18	309,59
Internal rent	**18,9**				
Current value	**0,000124701**		Goal seek:"Set cell d40 to 0 by changing		

3	4	5	6	7	8	9	10	
0,1280	0,1024	0,0819	0,0655	0,0524	0,0419	0,0336	0,0268	
							90,39053	
918,11	918,11	918,11	918,11	918,11	918,11	918,11	918,11	
422,55	422,55	422,55	422,55	422,55	422,55	422,55	422,55	
495,56	495,56	495,56	495,56	495,56	495,56	495,56	495,56	
231,40	185,12	148,10	118,48	94,78	75,83	60,66	48,53	
264,16	310,44	347,47	377,08	400,78	419,74	434,90	447,03	
73,97	86,92	97,29	105,58	112,22	117,53	121,77	125,17	
190,20	223,52	250,18	271,50	288,56	302,21	313,13	321,86	
231,40	185,12	148,10	118,48	94,78	75,83	60,66	48,53	
421,60	408,64	398,27	389,98	383,34	378,04	373,79	370,39	
-580,77	-172,13	226,14	616,12	999,46	1377,50	1751,29	2212,07	
0,5947	0,5001	0,4205	0,3536	0,2974	0,2501	0,2103	0,1768	
250,70	204,34	167,48	137,90	113,99	94,53	78,60	65,50	0,000125

g cell d37"

Table B.3: The table gives calculated amount of extra CH_4 [kg/h] for all six cases.

Case	Amount of CH_4 [kg/h]
Standard	3568
Hydrogen - Nitrogen ratio	4548
Steam-Carbon ratio	5333
Front-end pressure	5152
Mole fraction oxygen by membrane	4443
Mole fraction oxygen by electrolysis	4395

C   Mail correspondance - Haugland, Christer

Fra: Haugland,Christer <HAUGLAC@airproducts.com>
Sendt: 8. september 2016 13:35
Til: Henrik Jenssen Gremmetsen
Kopi: NODELAND,SVEIN G.; IHME,HANS
Emne: RE: Nitrogenproduksjon

Hei Henrik,

- Jeg har lagd en case basert på dine tall som du kan se på:
  - Produkt: 15 000 Nm3/h ved 95 vol% Nitrogen.
  - Luftbehov: 31 000 Nm3/h ved 9 barg. Har valgt 9 stk 450 kW oljesmurte skruekompressorer til dette.
  - Energibehov: rundt 870 kJ/Nm3 Nitrogen.
  - I vårt design bruker vi spillvarmen fra komprimeringen til å varme opp fødeluften inn på membranene til rundt 50 C. Har antatt dette designet i denne casen (utgjør i dette caset rundt 20 kJ/Nm3).
- Utløpstrykket varierer basert på bruken av nitrogen, men ligger typisk på 10-7 barg. Nitrogenet brukes ofte ved lavere trykk. Utløpstemperaturen er normalt 50-45 C.
- Energimengden som trengs for å produsere nitrogen er veldig avhengig av renheten du trenger på nitrogenproduktet. Dette gjelder spesielt membraner, men også PSA. Membraner er mest energieffektive ved lavere renheter. Er renhetskravet over 99 vol% er som regel PSA mer energigunstig. Med membranteknologi ligger hovedsaklig energibruken i komprimering av luft (det samme gjelder PSA).

Best regards,

Christer Haugland

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