Heat integration of the Haber Bosch process for the production of green ammonia

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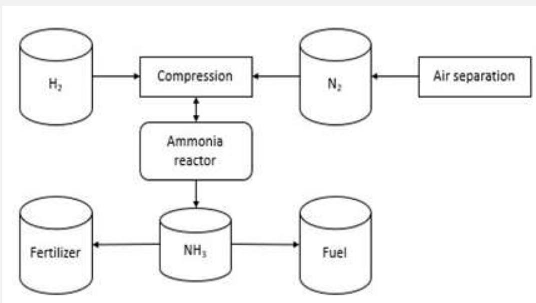

Ammonia is an important compound in the agricultural industry due to its large application in nitrogen-based fertilisers. The most common ammonia production pathway is the Haber – Bosch process, in which hydrogen from natural gas and nitrogen react. As natural gas prices keep rising and the decarbonisation of the chemical industry is required, it is important to start implementing large-scale green ammonia production processes [1].

A large-scale ammonia synthesis simulation was performed in *Aspen Plus,* which can be divided into two parts. An air separation unit that includes a compressor and two distillation columns to separate nitrogen from air, and a reactor for ammonia synthesis, which is separated from its reactants through two separators. An energy analysis was then performed in *Aspen Energy Analyzer*, with seven different types of utilities being used, and a heat exchanger network was created, in order to reduce the utilities spent and carbon emitted.

The results indicate process viability, with further optimization of the simulation and study of different ammonia synthesis techniques to be done in future work.

Introduction

The aim of this work was to simulate a large-scale ammonia production plant (500 thousand tonnes of ammonia per year) that improves upon the high energetic expenses related to the Haber – Bosch process. The simulation encompasses two different segments, an air separation unit and a reactor. An energy analysis for this process was made and optimization of the heat exchanger network was done through heat integration using *Aspen Energy Analyzer*. As one of the goals is to reduce environmental problems associated with the Haber – Bosch method, the simulated process' carbon emissions were also looked into before and after heat integration. The results will bring light to the viability of this alternative and the improvements to be made in order to maximize efficiency and minimize energy consumption.

Simulation

Air separation unit

The first module of this simulation is the air separation unit, where air enters at atmospheric pressure and temperature, and is compressed to 7 bar with further cooling to -200 ºC. These conditions guarantee that the air is fully liquified and ready to be separated into its components. Thus, two distillation columns were used sequentially to maximize separation efficiency, where nitrogen leaves as liquid distillate and oxygen as the bottoms product, with the nitrogen streams from each distillation column being mixed afterwards, as seen in the next Figure 1.

The columns were firstly simulated as DSTWU models, in order to obtain their reflux ratio and distillate to feed ratio. Then, the RADFRAC model was used and the main parameters were optimized through a sensitivity analysis, to maximize the separation efficiency.

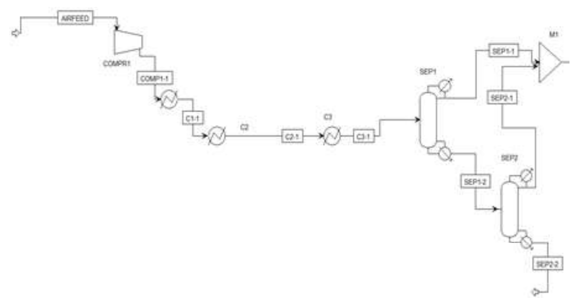

Figure 1. Diagram of the air separation unit.

Ammonia synthesis system

Furthermore, an independent hydrogen stream was mixed with the nitrogen obtained previously, which was then compressed to 128 bar through a series of compressors with coolers in between. This stream was then inserted into the reactor, where the ammonia formation reaction occurs.

$$\frac{1}{2}N_2 + \frac{3}{2}H_2 \rightleftharpoons NH_3 \qquad (1)$$

At 450 ºC and 128 bar, a conversion rate of 30% was considered for the ammonia production [2], and the reactor outlet was then cooled back to -30 ºC. Additionally, the cold stream was then separated into ammonia and the rest of the reagents, using two different flash separators, the first working at 128 bar, and the second at 17 bar.

The top stream of each separator is then mixed back before the reactor inlet, whilst guaranteeing that the mixture conditions are adequate, using multiple compressors and coolers to achieve the pre-reactor conditions. A purge is also necessary to guarantee that the air impurities are kept at a safe quantity. The full ammonia synthesis system is shown in Figure 2.

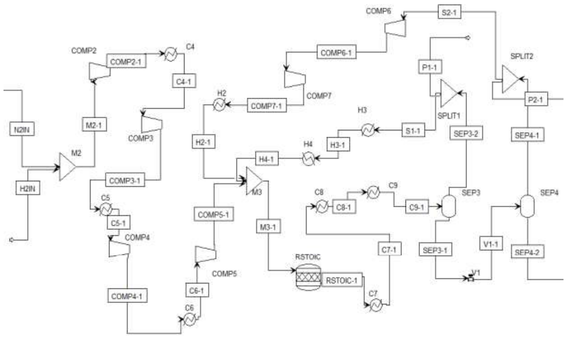

Figure 2. Diagram of the ammonia synthesis section.

Energy analysis

As mentioned previously, it is important to assess the energetic consumption of this process in order to understand its viability. Heat duties were obtained for each equipment and the electric consumption of pumps and compressors was calculated. Then, heat integration was performed in *Aspen Energy Analyzer* to create a heat exchanger network (HEN) that minimizes energy expenses and carbon emissions.

Results and conclusions

The simulation model presented in Figures 1 and 2 complied with the process specifications, producing 500 thousand tonnes of ammonia per year, with a molar purity of 98.3% and a global yield of 89.7 %. The main parameters for the air separation unit are also presented in the table below.

Table 9 – Main parameters of the distillation columns.

	SEP1	SEP2
Reflux ratio	1.37	6.00
Distillate to feed ratio	0.75	0.10
Number of stages	25.0	20.0
Feed stage	10.0	10.0
Efficiency (%)	96.0	99.7

Depending on the necessities of potential buyers, product purity could be improved upon, as well as total process yield, although at an increase in energy expended, which could be evaluated in the future.

An energy analysis of the process was also done, having utilized seven different types of utilities, which may be unnecessary and improved upon further. The heat exchanger network and the energy analysis's main results are described in Figure 3.

Table 2 – Energy analysis main results.

	Simulation
Total heat duty (MW)	407.6
Electrical consumption (MW)	65.8
Recoverable heat duty (MW)	108.1
Total utilities (GW)	284.2
Utilities after heat integration (GW)	133.3
Carbon emissions (kg/hr)	10490
Carbon emissions after heat integration (kg/hr)	-17970

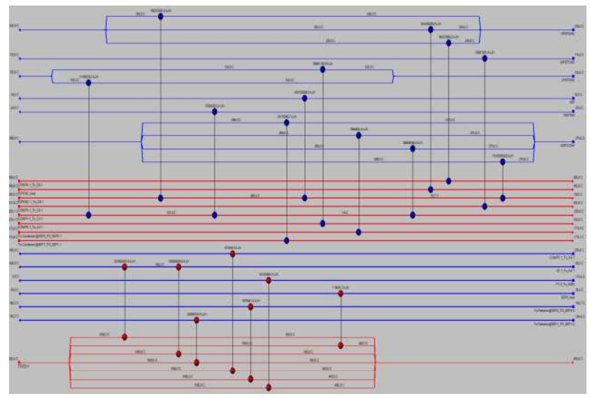

Figure 3. Diagram of the heat exchanger network.

These results are according to expectation, since the process is energetically intense and, according to Morgan et al. [3], a plant that produces 100 thousand tonnes of green ammonia per year has a heat requirement of around 150 MW. It is important to note that, after heat integration, the carbon emissions become negative, since there are three different types of steam being generated, whose impact is accounted for as avoided CO_2 emissions, and thus counts as negative emissions. Further investigation of this impact should be done in future work through life cycle assessment, to ensure that all sources of impact are being considered. Although water electrolysis has not been included in this simulation, its addition to the process in the future could be beneficial for research purposes. Different ammonia synthesis methods should also be investigated in order to maximize process efficiency and minimize energy consumption.

Acknowledgements

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