Heat Integration of the Haber Bosch Process for the Production of Green Ammonia

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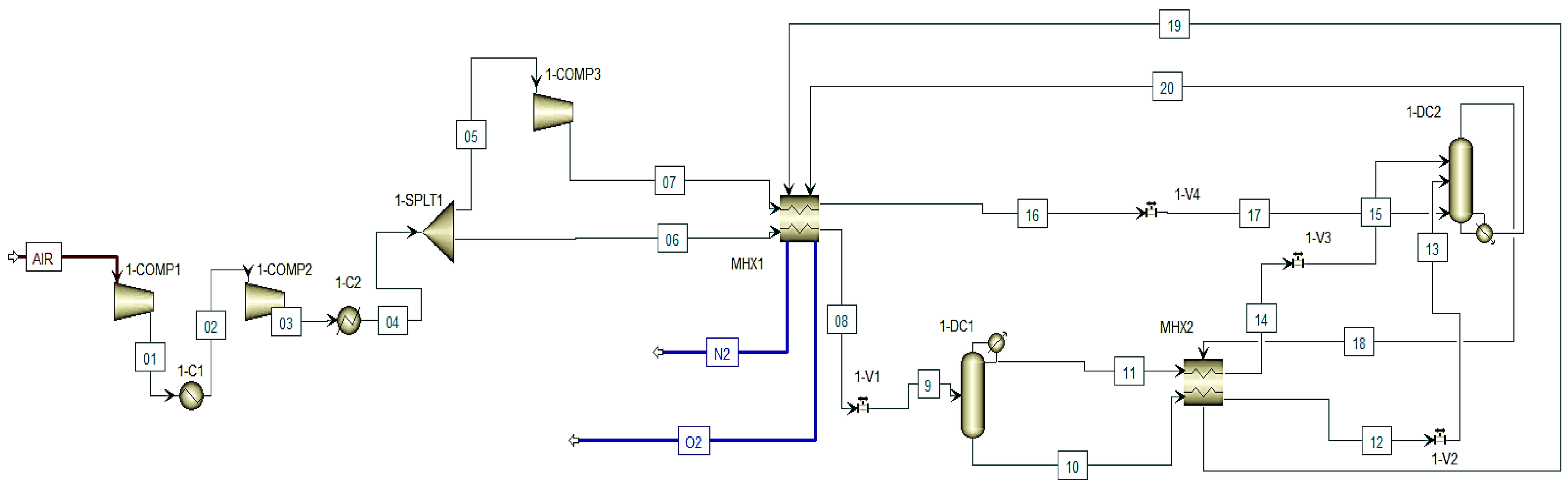
Introduction

- The **Haber-Bosch** (HB) process accounts for **over 1 %** of **total carbon emissions** whilst maintaining an extremely high energy consumption for a chemical process.
- Development and optimization of large-scale green ammonia production processes is **pivotal** to ensure **green ammonia** can substitute current ammonia synthesis processes .
- The aim of this work is to evaluate the **viability** of a large-scale green ammonia production plant and use **heat integration** to improve the energetic efficiency of this project.
- The simulation, developed in **Aspen Plus**, was divided into three different segments, an **air separation unit**, an **electrolyser** and the **ammonia synthesis** section.

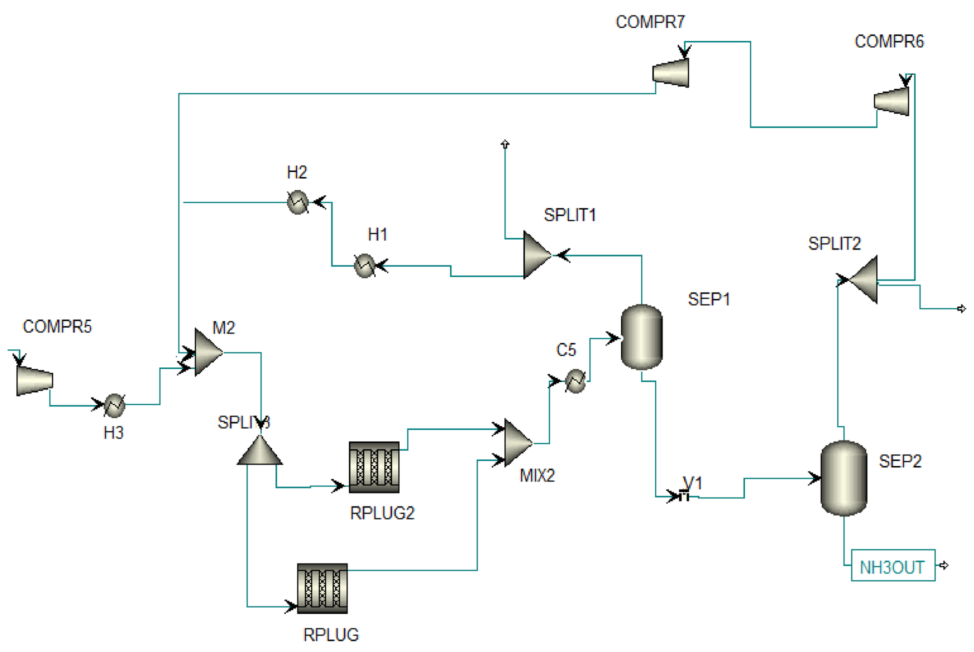
Air Separation Unit (ASU)

- Air is **compressed** and then **cooled** into **cryogenic temperatures** to facilitate the air separation through two different distillation columns.
- Nitrogen then leaves the ASU at atmospheric conditions, ready to be mixed with the hydrogen produced from the electrolyser.
- By varying the **temperature** outlets of the multi-heat exchangers and the **distillate rate** of the first distillation column:
  - **164 kt/year** of nitrogen were produced, with **99.1 % purity**.
  - A process **yield of 99.3 %** was achieved.



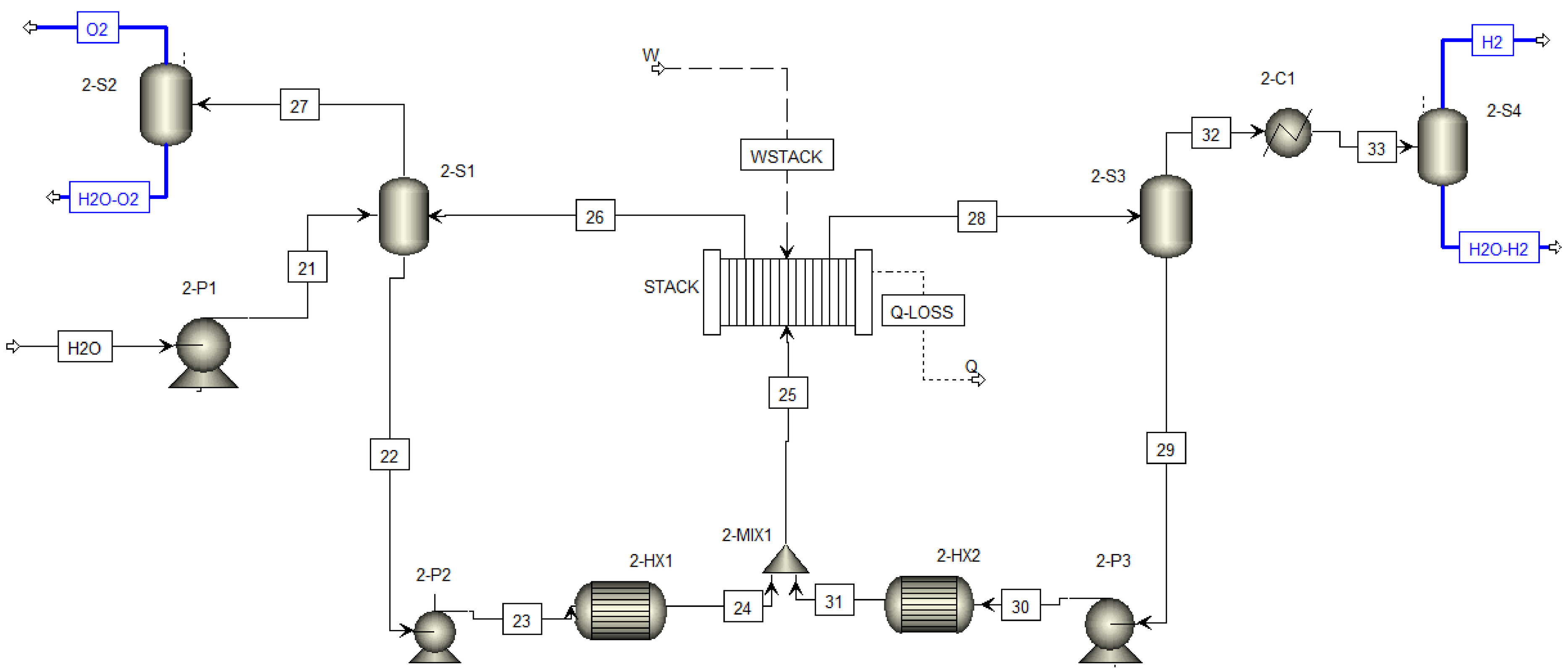
Ammonia Synthesis

- Nitrogen and Hydrogen are mixed and compressed to **128 bar** to allow ammonia synthesis.
- The reaction mixture is equally split into **two Plug Flow Reactors** to increase process robustness.
  - Conversion **increased** with catalyst loading
  - Optimum temperature of **450 °C** inside the reactor.
- The reactor outlets are then re – mixed and cooled to **cryogenic temperatures** to ensure that correct separation can occur.
- **200 kt/year** of green ammonia were produced, with **99.7 % purity.**



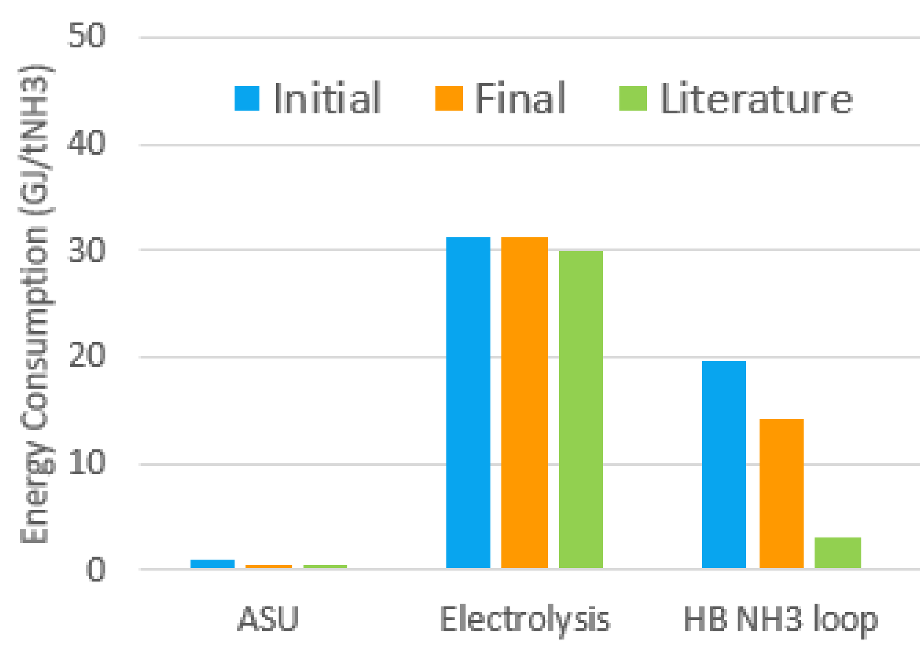
Electrolyser

- The electrolyser was modelled with *Aspen Custom Modeler*:
  - Pressure of **7 bar**.
  - Fraction of heat lost to surroundings fixed at **10%**.
  - Number of cells of the electrolyser established at **700 cells**, with each one having an area of **3** $\mathbf{m^2}$.
- Some notable results were:
  - A temperature of **135 °C** in the stack.
  - A Hydrogen to Oxygen (HTO) diffusion ratio **lower than 2 %**.
  - A hydrogen **purity** of **99.2 %**.
- The electrolyser has **200 MW** of power, leading to an annual production of **35 kt** of green hydrogen.



Heat Integration

- ASU energy consumption aligned with literature values.
- Electrolysis process scaled well.
- Heat integration was most useful for the NH_3 synthesis loops.
- Large inefficiencies regarding the NH_3 synthesis loops.



Conclusions and Future Work

- A large – scale green ammonia production plant was **developed successfully**, with its three main sectors working **efficiently**.
- The energetic consumption of the process is **promising**, however, further improvements are needed for the utility usage to improve upon the results obtained.
- To further reduce energetic expenses, an **absorbent – enhanced ammonia synthesis loop** was tested at a large scale, but the results were **not satisfactory**.
- An **economic evaluation** should be done as **future work**, alongside additional simulations on the **absorbent – enhanced process** at a large scale.

References

1. Rahman Daiyan *et al*, Nitrate reduction to ammonium: from CuO defect engineering to waste NOx-to-NH3 economic feasibility, Energy Environ. Sci. 14 (2021), 3588.
2. K.H.R. Rouwenhorst, A.G.J. Van der Ham, G. Mul, S.R.A. Kersten, Islanded ammonia power systems: technology review & conceptual process design, Renew. Sustain. Energy Rev. 114 (2019), 109339.

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