The impact of the hydrogen source on process conditions in ammonia production

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ABSTRACT

In the early 20th century, Fritz Haber and Carl Bosch succeeded in the development of a high pressure synthesis process that allowed the fixation of nitrogen from air in the form of ammonia. At the time, the source of hydrogen for this process was not important, resulting in processes operating with hydrogen obtained from coal gasification, natural gas reforming, or water electrolysis. Since then, ammonia's importance has grown significantly, as one of the most important chemicals in the world, with a strongly established role in the chemical industry for producing fertilizer and other nitrogen containing chemicals. In addition, ammonia has recently gained interest as a carbon free-fuel and an energy carrier, due to its relatively ease of transport with respect to hydrogen and an extensively developed ammonia infrastructure. Its production capacity is currently over 230 million tonnes per year and is expected to increase [1]. In the effort to phase out fossil fuels and transition to a carbon-free future, further confirmed by the COP28 [2], increased research attention has been also targeted toward shaping the hydrogen economy. In this context, ammonia production modelling with a focus on decarbonizing the production received significant attention in recent years.

Traditionally, ammonia production is studied in a coupled process that includes hydrogen production through steam reforming. Hence, depending on the included scope, it can be difficult to compare the individual reported values as well as apply them within energy system models studying the decarbonization of the complete energy system. In this work, we separate the ammonia production from the hydrogen production. Both hydrogen and nitrogen are produced separately and consequently mixed to produce the synthesis gas, with the advantage of increasing the flexibility with respect to the hydrogen source in the analysis. An especially important focus of this study is the changes in operating conditions depending on the hydrogen source. This is achieved through chemical process simulations in Aspen HYSYS. The process configuration and operating conditions have been selected through a systematic sensitivity analysis, focusing on how the energy consumption is affected by the purification section, different reactor layouts, and several separation configurations. The increasing complexity of the several options has also been considered, as it impacts the capital costs. The obtained process simulations allow us to study the impact of efficiencies, costs and lifetime for all technologies involved in the value chain, like different options for hydrogen production.

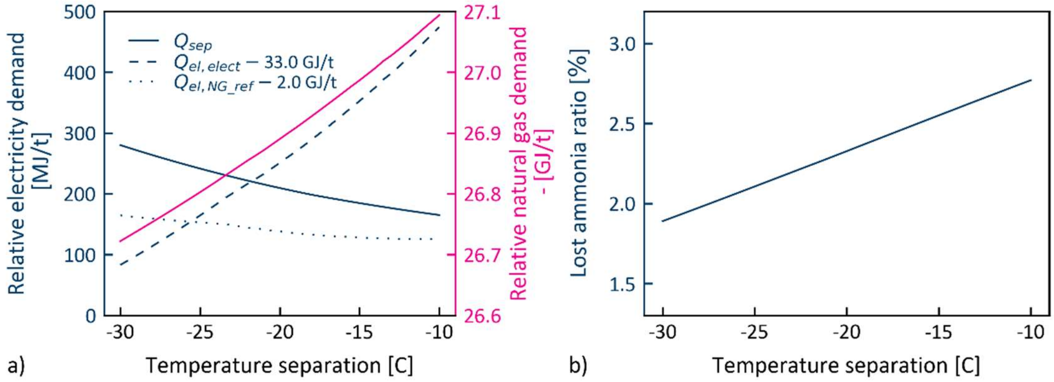

Figure 1: a) Relative electricity demand for the separation section, electrolysis-based ammonia (assuming an efficiency of 69 %), and natural gas-based ammonia (blue, [3]) and the relative natural gas demand for natural-gas based ammonia (LHV, red, [3]) as a function of the separation temperature, and b) loss of ammonia as a function of the separation temperature.

However, the relative electricity demand of the complete ammonia production only increases if hydrogen is produced from natural gas reforming. In the case of electrolysis-based ammonia, the total electricity demand is in fact decreasing due to a smaller loss of ammonia with a reduced separation temperature as outlined in Figure 1 b). This difference can be explained by the different energy sources used in natural gas-based hydrogen, where the total energy demand is also decreasing as shown by the relative natural gas demand. This highlights that the separation section has a major (indirect) impact on the energy demand of ammonia production, even though most of the publications on this topic neglect its detailed modelling.

As thermal energy has a different cost efficiency compared to electricity, switching from natural gas-based hydrogen to electrolysis-based hydrogen requires analysis related to the impact of chosen process parameters. Utilizing processes designed with natural gas-based hydrogen in mind without adjusting key process conditions would hence result in suboptimal performance with respect to production cost.

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