

Conversion of hydrogen to ammonia as a method of increasing energy density – a simulation study

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Abstract

In light of the current efforts of harnessing hydrogen as a potential carbon free energy source alternative to fossil fuels, ammonia has emerged as one of the possible candidates for an effective hydrogen storage method, due to its significantly simplified storage conditions. In this work, the Haber-Bosch process for ammonia synthesis was studied for three scales of production, in the aspect of energy efficient reactor design and optimal operational conditions, with the use of a process simulator, allowing for the manipulation of desired plant parameters in a wide range of values. Moreover, the energy balance of the process has been included in the research process allowing for the visualization of energetic cost of increasing the energy density of the system. The obtained data provides a basis for analysing the Haber-Bosch process in the context of ammonia conversion for hydrogen storage.

Keywords

energy density, ammonia synthesis, hydrogen storage, process simulation

1. INTRODUCTION

Ammonia has remained as one of the most important chemicals produced worldwide, owing to its key role in the manufacture of nitrogen fertilizers and, more recently, as a hydrogen and energy carrier. The global annual production of ammonia exceeds 200 Mt/year and relies almost exclusively on the Haber-Bosch process. This process consumes 1–2% of the world's total energy supply and 3–5% of global natural gas production (de la Hera et al., 2024). The associated CO₂ emissions are estimated at nearly 400 Mt/year. At such a large global production scale, even small relative improvements in process efficiency or carbon intensity translate into substantial absolute benefits. This makes the Haber-Bosch process an attractive subject for systematic simulation-based studies and justifies a critical review of existing modelling work across different production scales.

2. BACKGROUND AND LITERATURE REVIEW

This chapter summarises the current state of knowledge on the conversion of hydrogen to ammonia as a solution aimed at increasing the useful energy density of the system in energy storage and transport applications. The overview is organised into five subsections, which lead from a systemic perspective on the role of ammonia in energy systems and the power-to-ammonia

concept, through a reference to the industrial starting point of the Haber-Bosch process as a reference system and contemporary downscaling trends, to aspects key to simulation analyses: reactor and synthesis loop modelling, operating dynamics, and quantitative assessment of energy consumption and energy parameters in consistent kWh/kg NH₃ units.

2.1. Power-to-ammonia in energy systems

Ammonia is currently being analysed as an energy vector and part of the electricity-to-fuel/storage medium conversion chain in the power-to-ammonia concept, rather than solely as a chemical product (Jabarivelisdeh et al., 2022; Smith et al., 2020). This approach links NH₃ synthesis to the energy and emission balance of the entire system, in which the variability of energy supply (e.g. from renewable energy sources) forces the process to be evaluated under dynamic conditions and partial loads (Fahr et al., 2025; Smith et al., 2020; Verlysen et al., 2021). Small-scale energy-oriented analyses show that in P2A (Power to ammonia) it is crucial to break down energy consumption into stages (H₂ production, N₂ production, synthesis loop) and to assess the efficiency-flexibility-unit cost trade-off (de la Hera et al., 2024; Lin et al., 2020). From an implementation perspective, it is also important to determine the safe operating range and flexibility constraints resulting from the apparatus and thermodynamics of the Haber-Bosch loop (Cheema and Krewer, 2018; Fahr et al., 2025).



2.2. Haber–Bosch: reference and downscaling

Classic large-scale installations serve as a reference system for assessing the energy efficiency, stability and maturity of technological solutions, as illustrated by the description of a large scale installation based on proven technology (Rüther et al., 2005). In this approach, the synthesis loop (compression, multi-bed reactor, recirculation, NH_3 separation) is treated as a reference system for loss analysis, optimisation and control solution design (Araújo and Skogestad, 2008; Flórez-Orrego and de Oliveira Junior, 2017; Luyben, 2012). At the same time, pressure to integrate with non-stationary energy generation and to lower investment barriers is driving research towards small scale, modularity and continuous operation as a design paradigm for installations adapted to distributed power supply (Garrote, 2020; Seifert et al., 2012). In this trend, techno-economic and energy analyses of small-scale methods based on Haber-Bosch technology point to a change in the cost and energy structure and to sensitivity to the choice of loop configuration and operating conditions (de la Hera et al., 2024; Lin et al., 2020). At the same time, concepts for process intensification are being developed as a 'bridge' between the classic system and distributed production, in which the reorganisation of heat exchange and the densification of equipment have the potential to reduce scale limitations (Garrote, 2020; Spatolisano and Pellegrini, 2023).

2.3. Reactor and synthesis loop: modelling and dynamics

Modelling based on differential equations forms the basis for describing the synthesis reactor and the entire loop, from stationary models to dynamic and optimisation analyses (Amin et al., 2013; Dashti et al., 2006; Flórez-Orrego and de Oliveira Junior, 2017). Reactor models (most often similar to Plug Flow Reactor – PFR with heterogeneous kinetics) allow quantitative investigation of the influence of temperature, pressure and composition on conversion and on temperature distributions determining cooling requirements (Amin et al., 2013; Dashti et al., 2006; Shamiri and Aliabadi, 2021). An exergetic approach to modelling and optimising industrial units allows the identification of loss locations and the interpretation of limitations to energy efficiency improvements (Flórez-Orrego and de Oliveira Junior, 2017).

In industrial practice, a 3-bed reactor is commonly used, in which the exothermicity of the equilibrium reaction requires controlled heat removal between the beds, which ensures that the temperature is maintained within the catalyst activity window and limits the decrease in thermodynamic drive (Luyben, 2012; Rüther et al., 2005). 3-bed configurations differ primarily in the method of heat removal: interstage cooling using inter-bed exchangers or cooling by injecting cold gas (quench) between the beds (Luyben, 2012; Rosbo et al., 2023). Comparisons of reactor configurations in terms of cooling methods

indicate that the method of heat removal affects the temperature distribution in the beds, conversion and intensification potential (Khademi and Sabbaghi, 2017). Design and control analyses of the cooled reactor show a strong coupling between temperature profile, chemical equilibrium and operational stability, making heat removal a critical degree of design freedom (Luyben, 2012; Shamiri and Aliabadi, 2021).

Flexible operation of the Haber–Bosch loop requires dynamic tools, as the process is non-linear and prone to instability phenomena (Morud and Skogestad, 1998; Verlysen et al., 2021). Reactor instability mechanisms and their consequences for the selection of controlled variables are a classic starting point for designing synthesis loop control structures (Araújo and Skogestad, 2008; Morud and Skogestad, 1998). In P2A terms, dynamic sensitivity analysis and stabilisation strategies (including for a quench reactor) indicate that the selection of operating trajectories, equipment limitations and anti-surge requirements affect the achievable load range and transient responses (Rosbo et al., 2023; Verlysen et al., 2021). Dynamic simulations of high load flexibility installations show that power consumption and loop conditions vary with load, and the ability to reduce pressure and compression power depends on the operating strategies adopted (Fahr et al., 2025). Determining the safe operating area for P2A designs formalises the operating constraints that determine the acceptable range of parameters and system stability (Cheema and Krewer, 2018).

2.4. H_2 to NH_3 conversion: energy and energy density (kWh/kg NH_3)

In analysing the increase in 'system energy density' through H_2 to NH_3 conversion, it is crucial to distinguish between the energy chemically stored in NH_3 and the energy expenditure of conversion throughout the P2A chain (Jabarivelisdeh et al., 2022; Smith et al., 2020). Smith et al. (2020) assume a lower limit for the energy 'contained' in the carrier equal to the Lower Heating Value (LHV) of ammonia, 5.17 kWh/kg NH_3 . Jabarivelisdeh et al. (2022) use an energy value of 5.75 kWh/kg NH_3 for the product for their production pathway comparisons (Jabarivelisdeh et al., 2022). Smith et al. (2020) also give the LHV energy of the stoichiometric amount of hydrogen needed to produce 1 kg NH_3 as 5.92 kWh/kg NH_3 , which is the reference point for the energy balance of the conversion.

The energy cost of conversion in an electrified chain strongly depends on the stage of H_2 production, as confirmed by literature balances (Lin et al., 2020; Smith et al., 2020). For the electrolysis-based variant (60% efficiency). Smith et al. (2020) report a total energy demand of 10.61 kWh/kg NH_3 , of which 9.86 kWh/kg NH_3 is accounted for by H_2 production and approximately 0.75 kWh/kg NH_3 by N_2 separation and compression in the synthesis loop (Smith et al., 2020). In the same study, the reference ranges for best available techniques (BAT) are 7.61–8.83 kWh/kg NH_3 , which allows P2A assessments to be set against industrial energy benchmarks (Smith et al., 2020).

On a small scale, [Lin et al. \(2020\)](#) report total energy consumption of 9.36–9.70 kWh/kg NH₃ for the all-electric configuration, with energy attributed to the synthesis loop alone of 0.37–0.71 kWh/kg NH₃, which explicitly separates the energy cost of NH₃ production from the cost of the Haber–Bosch part. For the reference large-scale case based on SMR, [Lin et al. \(2020\)](#) report a total consumption of 8.89 kWh/kg NH₃, and an energy consumption of the synthesis loop alone of 1.28 kWh/kg NH₃, which serves as a reference point for scale and configuration comparisons.

[De la Hera et al. \(2024\)](#) present small-scale energy simulations directly in P2A logic, reporting a total consumption of 214–217 kWh/kmol NH₃, which corresponds to 12.57–12.74 kWh/kg NH₃ after conversion. The authors also provide a share distribution of energy consumption, which is dominated by electrolysis (e.g. ~ 80.6%), with a significant share attributable to H₂ synthesis (~ 18.6%) and N₂ production having a marginal share (~ 0.818%), which supports the analysis of the energy expenditure structure in P2A ([de la Hera et al., 2024](#)).

2.5. Summary of the literature collection

The literature review forms a coherent chain of argumentation: systemic and energy-emission studies place P2A in the context of energy balance and the role of NH₃ as a carrier ([Jabarivelisdeh et al., 2022](#); [Smith et al., 2020](#)), while classic large-scale technology provides a reference system for design and control solutions ([Araújo and Skogestad, 2008](#); [Rüther et al., 2005](#)). Development trends towards small scale, modularity and intensification require an assessment of the flexibility-energy trade-off ([de la Hera et al., 2024](#); [Garrote, 2020](#); [Lin et al., 2020](#); [Seifert et al., 2012](#); [Spatolisano and Pellegrini, 2023](#)). The methodological core remains reactor and loop modelling (stationary and dynamic) and operational stability analysis, which determine whether energy consumption reduction is achievable in the real P2A operating area ([Amin et al., 2013](#); [Cheema and Krewer, 2018](#); [Dashti et al., 2006](#); [Fahr et al., 2025](#); [Flórez-Orrego and de Oliveira Junior, 2017](#); [Khademi and Sabbaghi, 2017](#); [Luyben, 2012](#); [Morud and Skogestad, 1998](#); [Rosbo et al., 2023](#); [Shamiri and Aliabadi, 2021](#); [Verlysen et al., 2021](#)).

This study analysed simulation performance under operating conditions such as ammonia production intensity, including simultaneous changes in key process variables such as reactor pressure, ammonia concentration in the recirculation/feed stream, H₂ to N₂ molar ratio, total feed mass flow rate, and reactor inlet temperature, while tracking energy consumption consistently across the entire operating range.

In addition, special case studies were conducted on changes in parameters such as reactor pressure, ammonia concentration in the feed loop, H₂ to N₂ molar ratio, total feed mass, and reactor inlet temperature, and the results obtained were compared with those reported in the literature for all operating ranges.

Table 1 presents selected production scale values. [Lin et al. \(2020\)](#) analyzed two conceptual variants of the process. In two configurations, a high-pressure reactor operating at 200 bar was used, and the product was separated by condensation (RXN–CON system, i.e. reactor–condenser). In the variant by ([Lin et al., 2020](#)), on the other hand, the reactor operates under low pressure (8 bar), and the product is obtained in liquid form through absorption. In contrast, in [Garrote \(2020\)](#) production was divided into four scales: 75%, 50% and 25% of the nominal production of 45540 kg/h of ammonia. A multi-tube reactor was used in each of them, with 250, 200, 150, and 100 tubes, respectively, depending on the scale of production.

Table 1. Scope of literature overview on ammonia synthesis using the Haber–Bosch process.

Order ID	Source	Method	Reactor type	NH ₃ production, kg/h
1	Spatolisano and Pellegrini, 2023	AS	3BR–AIIC	9350
2	Rosbo et al., 2023	MM	3BR–AQCR	4031
3	Shamiri and Aliabadi, 2021	MM	3BR–AQCR	20083
4	Verlysen et al., 2021	AS	FR–1	80
5a	Garrote, 2020	AS	FR–250	45540
5b	Garrote, 2020	AS	FR–200	34155
5c	Garrote, 2020	AS	FR–150	22770
5d	Garrote, 2020	AS	FR–100	11385
6a	Lin et al., 2020	AS	3BR–AQCR	2284
6b	Lin et al., 2020	AS	3BR–AQCR	2428
7	Cheema and Krewer, 2018	MM	3BR–AQCR	100
8	Flórez-Orrego and Oliveira, 2017	AS	3BR–AIIC	41667
9	Luyben, 2012	AS	3BR–AQCR	71053
10	Araújo and Skogestad, 2008	AS	3BR–AQCR	70958

Abbreviations: AS – Aspen simulation; MM – mathematical model; FR–x – flow reactor, where x is number of tubes; 3BR – 3-bed reactor; AQCR – adiabatic quench cooled reactor; AIIC – adiabatic indirect intercooling.

3. SIMULATION MODELS AND METHODS

In this project, AVEVA Process Simulation is used to model ammonia synthesis. The first step, before beginning work on the simulation, was a selection of suitable thermodynamic model for the considered conditions and substances. A preliminary selection was made, leaving only models that were not limited by high temperatures (350–500°C) and pressures (150–250 bar) of the Haber Bosch process. A particularly important

part of the simulation that is highly dependent on the chosen model is the product separation through condensation, as then the system functions in the vapour-liquid equilibrium (VLE). Two chosen thermodynamic models: Soave–Redlich–Kwong (SRK) and Soave–Redlich–Kwong Modified Panagiotopoulos–Reid (SRKM), were compared to the experimental data of VLE equilibrium of a three component, $\text{NH}_3\text{--H}_2\text{--N}_2$ system with considered ammonia concentrations (10% and 20%) (Michels et al., 1950). The results have been shown in Figure 1.

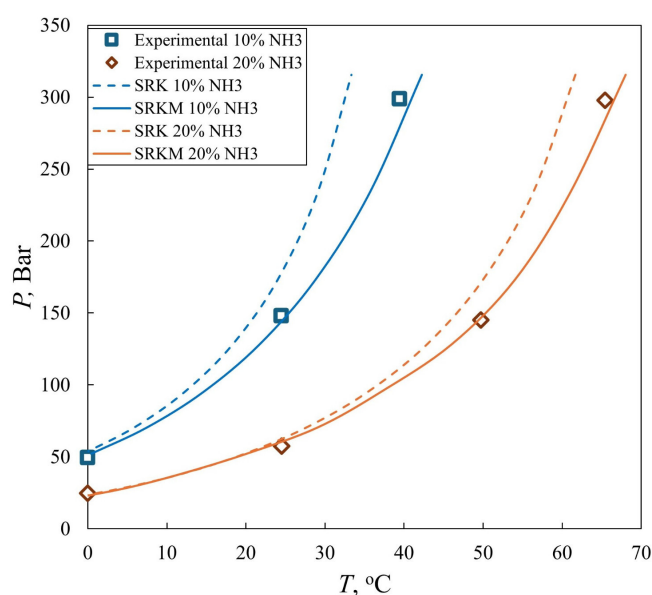


Figure 1. Comparison of experimental data (Michels et al., 1950) and two thermodynamic models (SRK, SRKM) for two ammonia concentrations as a PT curve.

Based on the data presented in Figure 1, the SRKM model has proven to be a better candidate for the considered process. The model improves the accuracy of predictions for strongly asymmetric mixtures of polar and nonpolar components compared to the SRK model, by using an asymmetric mixing rule (AVEVA™ Process Simulation, 2025). The model is described by Eq. (1):

$$P = \frac{RT}{V - b} - \frac{a(T)}{V(V + b)} \quad (1)$$

where a and b are parameters specific to the considered system, defined by Eq. (2) and Eq. (3) respectively:

$$b = \sum_i x_i \frac{0.08664RT_{c,i}}{P_{c,i}} \quad (2)$$

$$a(T) = \sum_i \sum_j x_i x_j a_{ij} \quad (3)$$

The prepared simulation has been split into 3 sub-flowsheets using the *Flag* model. This solution has several benefits, it is used not only to improve the convergence of recycles through iterative sequential updates, rather than by solving it simultaneously, but it also makes the simulation clearer, splitting it visually into smaller subsections. The considered

subsections are: Feed preparation, Reactor, and Condensation and Recycle, which have been discussed in further detail in their own sections.

3.1. Feed preparation

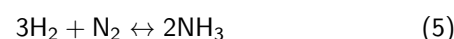
In the prepared simulation, the AVEVA naming convention has been utilized. Each element was given a name according to the formula: A_B, where A is the subsection code: S – substrate preparation section, R – reaction section, M – main condensation and recycle section, and B is the name of the model: S – stream, XV – valve, V – drum, K – compressor, HDR – junction, R – reactor bed, E – heat exchanger.

Figure 2 depicts the first part of the simulation involving the compression and heating of the substrates before their mixing.

The hydrogen and nitrogen feeds are correlated with the molar ratio expressed by Eq. (4):

$$R_{\text{H}_2/\text{N}_2} = \frac{F_{\text{S_H}_2}}{F_{\text{S_N}_2}} \quad (4)$$

where $F_{\text{S_H}_2}$ and $F_{\text{S_N}_2}$ are the molar streams of hydrogen and nitrogen, respectively. This approach has several advantages. The equation allows hydrogen mass flow to be the only variable necessary for analysing the capacity of the installation. Additionally, the $R_{\text{H}_2/\text{N}_2}$ coefficient in the equation was used as a changing parameter in the following case studies to demonstrate the influence of the ratio of the hydrogen and nitrogen flow on the selected observed parameters. The value of the coefficient has been chosen based on the stoichiometry of the reaction, Eq. (5), with slight positive and negative deviations in the case study, i.e. varying between 2.8 and 3.2:



$$\Delta H = -46.2 \left[\frac{\text{kJ}}{\text{mol}_{\text{NH}_3}} \right] \quad (6)$$

The hydrogen source in the simulation had no impurities and the studied mass flow rates in the simulation were chosen and tuned based on the desired product flow rate. The ammonia synthesis process is sensitive to impurities that are present in air like oxygen or carbon oxides. The impact of impurities on the process was not the focus of this work. That is why the nitrogen source consisted of 100% pure nitrogen.

Both substrates are firstly inserted into buffer tanks through valves that are used to calculate the pressure drop. Next, a series of compressors (S_K1-3) heighten the pressure of the gases to the desired amount, i.e. 200 bar. For the hydrogen stream, an additional heat exchanger S_E1 is also needed as an in-between cooling step. The gases are then combined in the S_HDR1 junction and the mixture is transported to the next part of the simulation with the use of *Flag 1*, which has been used in order to visually split the simulation into multiple smaller regions, while improving the integrity of numerical calculations.

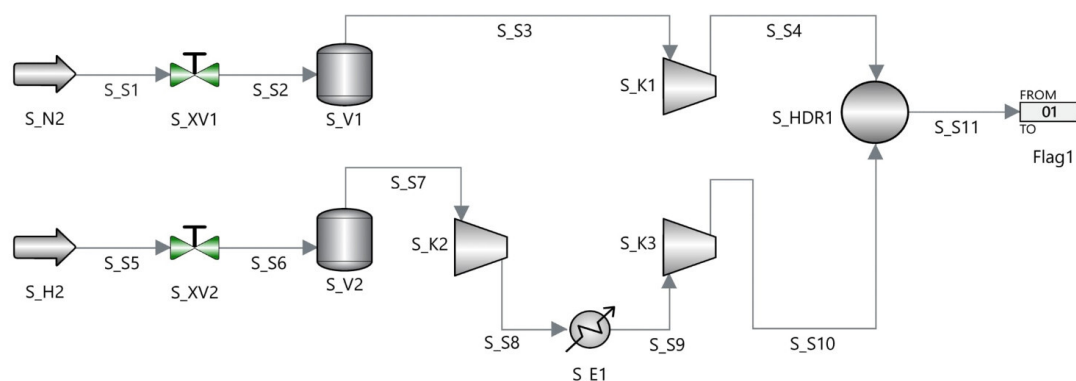


Figure 2. Source section: preparation of the nitrogen and hydrogen streams.

3.2. Reactor

Currently, the standard design solution in ammonia synthesis via the Haber–Bosch process is a three-bed reactor. The catalytic bed is divided into three consecutive reaction sections, separated by cooling zones and by throttling/flow-distribution elements. This architecture enables the temperature to be maintained within limits acceptable for both the catalyst and the equipment, while allowing operation as close as possible to the thermodynamic optimum (a compromise between reaction kinetics and equilibrium constraints). The three-bed configuration constitutes a common starting point both for stability and control analyses of the ammonia converter (Morud and Skogestad, 1998) and for studies aimed at increasing the flexibility and energy efficiency of the Haber–Bosch synthesis loop (Araújo and Skogestad, 2008; Rosbo et al., 2023).

In industrial practice, two dominant approaches to temperature control in three-bed systems are employed. The first, most commonly used, is the AQCR (adiabatic quench cooled reactor) concept, in which interstage cooling is achieved by mixing the hot post-reaction gas with a stream of “cold” synthesis gas (quench) prior to feeding the mixture to the next catalytic bed. The second approach is adiabatic indirect cooling, which involves heat removal in a heat exchanger integrated into the reactor or located externally (external interstage coolers). In both cases, the objective is to limit the temperature rise associated with the strongly exothermic nature of ammonia synthesis and to maintain a favourable temperature profile along successive bed sections.

In this work, Figure 3, the AQCR variant was selected due to its advantageous engineering features: simpler mechanical implementation (no additional heat-exchange equipment in the interstage line), reduced capital expenditures, and lower cooling energy demand owing to the use of a lower-temperature base stream as the quench medium.

For simulation purposes, the three-bed reactor was represented as a series of three tubular reactors (R1–R3) corresponding to

the three catalytic-bed sections, with interstage cooling implemented in mixing headers (nodes combining the post-reaction stream with the quench feed). Fresh synthesis gas is supplied from node Flag1 (graphical representation of data from stream S_S11 from the source section in Figure 2) and then mixed in the header with the recycle gas stream Rcy1. In the industrial plant, the start-up heat exchanger is installed upstream of the header to preheat the feed during start-up. This unit was omitted from the simulation flowsheet because, under steady-state operation, its contribution to the overall energy balance is omitted since the required preheating of the mixture upstream of the first bed is provided by the recycle stream, and the calculated heat duty of the start-up exchanger approaches zero.

In the presented simulation, the conversion of substrates to ammonia was kept at around 20%. However, in the literature the conversion values varied between 14.4 % and 30% as reported in Table 2. In an article Cheema and Krewer (2018) reported a conversion rate closer to the higher range of values reaching a result of 24.5%. In the work of Smith et al. (2020), due to the use of a ruthenium (Ru) catalyst (the process temperature is relatively lower, ranging from 573.15 K to 673.15 K). However, in (Shamiri and Aliabadi, 2021), optimisation of the conversion process increased it from 15.24 to 15.45%.

Table 2. Conversion values per one reactor pass reported in literature.

Publication	Conversion [mol. %]	Pressure range [bar]	Temperature range [°C]
de la Hera et al., 2024	14.4–23.8	160–295	350–540
Smith et al., 2020	15	150–250	300–400
Shamiri and Aliabadi, 2021	15.45	87.2	358–466
Cheema and Krewer, 2018	24.5	200	350–500
Jabarivelisdeh et al., 2022	20–30	100–250	350–550

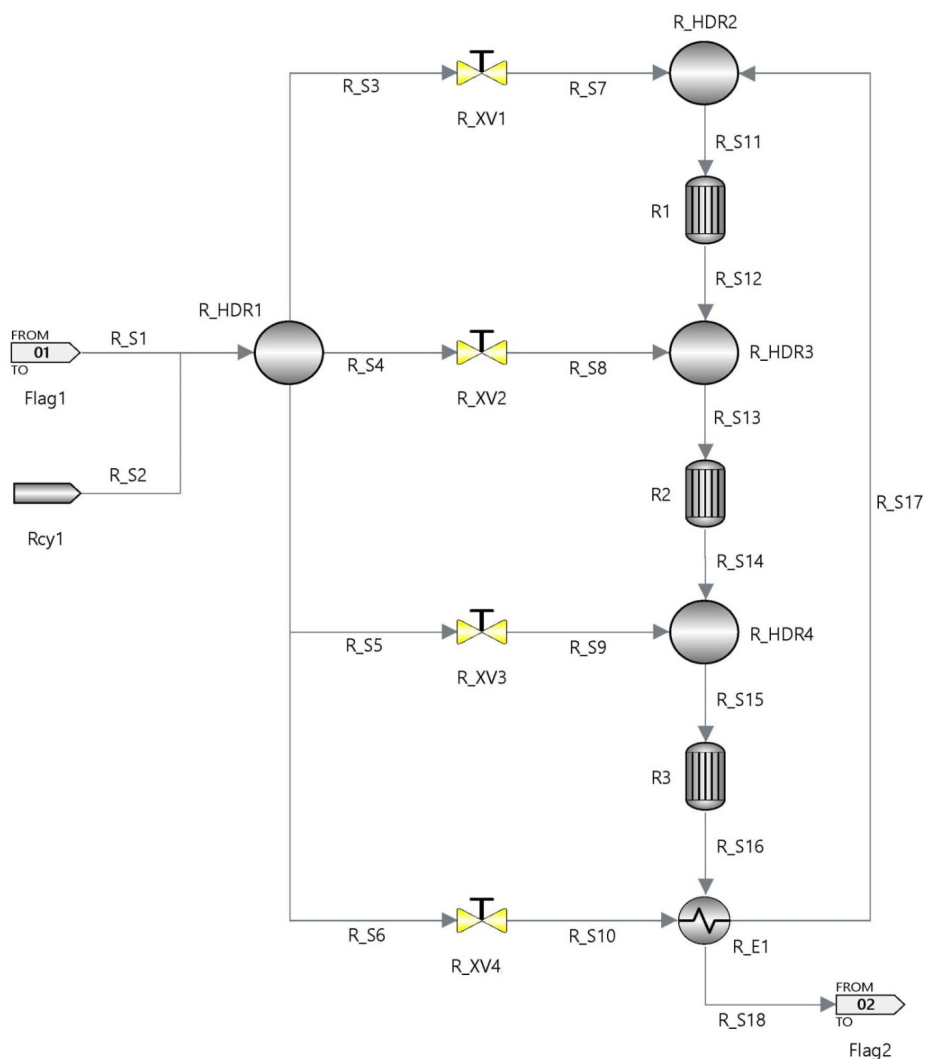


Figure 3. Reaction section: representation of adiabatic quench cooled reactor in process simulator.

An analysis of available models of three-bed ammonia synthesis reactors shows that both industrial and small-scale units employ strictly increasing volumes of consecutive catalyst beds. For reactors with constant diameter, typical volume ratios fall within the ranges: ($V_1/V_3 = 0.35\text{--}0.5$) and ($V_2/V_3 = 0.6\text{--}0.7$). The reactor sizes reported in the literature along with the production scales have been shown in Table 3.

Based on these observations, a unified, dimensionless description of bed size was adopted in this work, in which the volume of the third bed is used as a reference ($V_3 = 100\%$). The volumes of the other two beds are defined as fixed fractions of V_3 :

$$V_1 = 0.35 \cdot V_3 \quad (7)$$

$$V_2 = 0.65 \cdot V_3 \quad (8)$$

The choice of 35–65–100 proportions correspond to the lower bounds of the ranges reported in the literature (Araújo and Skogestad, 2008; Fahr et al., 2025; Lin et al., 2020; Morud and

Table 3. Relative size of catalytic beds.

Source	V_{1BR} [m ³]	V_{2BR} [m ³]	V_{3BR} [m ³]	Ratio of $V_{1BR} : V_{2BR} : V_{3BR}$
Fahr et al., 2025	17.1	27.9	43.4	39:64:100
Shamiri and Aliabadi, 2021	12.7	22	32	40:69:100
Morud and Skogestad, 1998	6.69	9.63	15.2	44:63:100
Araújo and Skogestad, 2008	6.69	9.64	15.2	44:63:100
Rosbo et al., 2023	1.4	2	3.2	43:63:100
Lin et al., 2020 RXN-ABS variant	1	2	3	33:67:100
Lin et al., 2020 RXN-CON variant	0.5	0.7	1	50:70:100

Skogestad, 1998; Rosbo et al., 2023; Shamiri and Aliabadi, 2021) included in Table 3. On the one hand, this preserves consistency with industrial solutions; on the other, it helps to reduce the overall pressure drop while maintaining a large completing volume in the third bed (Dashti et al. 200; Khademi and Sabbaghi 2017; Luyben, 2012; Shamiri and Aliabadi 2021).

Table 4 summarises the adopted values of individual bed volumes for selected reactor configurations.

Table 4. Size of bed's reactor in this work.

Production [t/h]	V _{1BR} [m ³]	V _{2BR} [m ³]	V _{3BR} [m ³]	D [mm]	L/D [m/m]
0.3	0.12	0.23	0.35	500	7.2
11.5	4.76	8.85	13.61	1700	7.1
23	9.09	16.88	25.96	2100	7.1

The smallest production scale considered, 300 kg/h of NH₃, was selected as potentially feasible in a containerised installation, assuming a modular layout and scalability by adding identical modules. The dimensions of the individual beds were determined based on literature data, adopting 35% and 65% of the volume of a three-bed reactor (3BR), respectively. The production level of 23000 kg/h NH₃ was selected – in line with the findings of (de la Hera et al., 2024) – as economically most favourable, whereas 11500 kg/h NH₃ serves as an intermediate scale, linking the container-level installation concept with the largest case under consideration.

3.2.1. Catalyst

The most commonly used catalysts are amorphous materials based on iron with various additives, including K₂O, Al₂O₃, and CaO, several also contained cobalt as one of the dopants (AntenChem, 2025; Syamcat, 2026). The parameters of commercially available ammonia synthesis catalysts are listed in Table 5.

Table 5. Parameters of commercially available catalysts used in ammonia synthesis.

Source	Chemical composition	ϵ [m ³ /m ³]	ρ_p [kg/L]	ρ [kg/L]	d_{cat} [mm]	T_o [°C]	p_o [MPa]
Zhulin Carbon, 2010	Fe ₃ O ₄ , K ₂ O, Al ₂ O ₃ , CaO, MgO	0.46	2.8–3.0	n.s.	1.5–9.4	500	n.s.
Syamcat, 2026	Fe–Co	0.45	2.4–3.2	n.s.	1.5–13	n.s.	n.s.
AntenChem, 2025	Fe ₃ O ₄ , K ₂ O, Al ₂ O ₃ , CaO, Co ₃ O ₄	0.45	2.2–3.0	n.s.	1.5–3.0	n.s.	n.s.
Dengzhuochem, 2025	Fe ₃ O ₄ , K ₂ O, Al ₂ O ₃ , CaO	n.s.	2.3–3.2	n.s.	1.5–3.0	350–530	10–40
Stanford Advanced Materials	Fe _(1-x) O, Al ₂ O ₃ , K ₂ O, CaO	n.s.	3.0–3.4	n.s.	1.5–13	330–500	10–32
Catalystzeolite, 2025	Fe ₃ O ₄	0.46	2.2–2.4	3.5–3.6	1.5–13	350–500	10–31.4

Abbreviations: n.s. – not specified.

The porosity and grain size of the catalyst are needed for the calculation of pressure drop in the reactor. In the simulation, the Ergun pressure drop model was chosen to calculate the pressure drop ΔP of gas flowing through a catalytic bed. The model is described by the equations:

$$1000 \cdot \Delta P_{elem} = \left(\frac{150 \cdot \mu \cdot v \cdot (1 - \epsilon)^2}{d_{cat}^2 \cdot \epsilon^3} + \frac{1.75 \cdot \rho \cdot v \cdot |v| \cdot (1 - \epsilon)}{d_{cat} \cdot \epsilon^3} \right) \cdot L_{elem} \quad (9)$$

$$v \cdot \rho \cdot \left(\frac{\pi}{4 \cdot D^2} \right) = F \cdot MW \quad (10)$$

The objective of the aforementioned equations is to calculate the pressure drop of the catalytic bed by summing the calculated pressure drop of each individual submodel. Eq. (9) is the core element and is known as the Ergun equation (Esence et al., 2017). Its result – the pressure drop of the discrete element of the catalytic bed – is the outcome of summing the viscous and inertial terms inside the parentheses. Eq. (10) shows a basic correlation between variables by equating two formulas for mass flow rate, which the program uses to lower the degrees of freedom.

For the simulation, a porosity of 0.45 and a catalyst diameter of 3 mm – the most common value offered by catalyst suppliers (Table 5) – were chosen to calculate the pressure drop. Packing density is a parameter that is heavily dependent on catalyst particle size. It takes on a wide range of values. However, the parameter needed for the calculation of the pressure drop through the Ergun model is particle density, which is why a value of 3500 kg/m³ was chosen. Operational temperature and pressure are the conditions under which the catalyst is active. They were taken into consideration while planning the flow rates and temperatures of the gases delivered into the reactor. Iron-based ammonia synthesis catalysts are also sensitive to impurities, particularly oxygen and carbon oxides,

which may contaminate the source gas streams. However, the effect of impurities was not the focus of this work, which is why pure nitrogen and hydrogen were chosen as substrates.

3.2.2. Reaction kinetics

The Temkin and Pyzhev model (Temkin and Pyzhev, 1940) was chosen as the model describing the heterogeneous reactions occurring on the surface of the iron catalyst. The model is suited for high-pressure, high-temperature reactions with VLE equilibrium, which are the characteristics of the process that is the focus of this work. The reaction rate of the model is described as the difference between the rate of the ammonia synthesis reaction and the ammonia decomposition reaction, which depend on the partial pressures of the gas mixture components. The denominator of the fractions has been increased by the value of 10^{-5} in order to prevent numerical errors when partial pressures of either ammonia or hydrogen reach the value of zero. The following semi-empirical Eq. (11) shows the method of calculating the reaction rate:

$$r = \frac{k_1 \cdot p_{N_2} \cdot p_{H_2}^{1.5}}{p_{NH_3} + 10^{-5}} - \frac{k_2 \cdot p_{NH_3}}{p_{H_2}^{1.5} + 10^{-5}} \quad (11)$$

The classic Arrhenius equation was used to calculate the reaction rate constants k_1 and k_2 . The pre-exponential constant A_i and the activation energy E_i have been chosen according to Table 6:

$$k_i = A_i \cdot \exp\left(-\frac{E_i}{RT}\right) \quad (12)$$

Table 6. Parameters in the Arrhenius equation (AVEVA™ Process Simulation, 2024).

i	A_i	E_i , kJ/mol
1	5	87.3
2	$7.02 \cdot 10^{12}$	200

3.3. Condensation and recycling

Figure 4 shows the section representing the condensation and recycle stream to the reactor section. The process has been described in more detail in Sections 3.3.1 and 3.3.2.

3.3.1. Condensation

The third subsection of the simulation begins with model *Flag2*, importing data from the Reactor sub-simulation described in the previous section. To condense ammonia, the high-pressure cooling method has been chosen, in which the gaseous mixture is cooled down, first in the exchanger M_E1 and later in the drum M_V1. The reaction product is separated from the unreacted gases and uncondensed leftover ammonia at 25 °C. The condensation parameters have been analysed based on phase diagrams of a mixture of ammonia and the unreacted hydrogen and nitrogen with the molar ratios corresponding to the ratios at the outlet of the reactor. Condensation pressure is dictated by the outlet reactor pressure and in the considered process is equal to around 200 bar. During the process of condensation, the ratios between the ingredients of the vapour phase change, as the less volatile ammonia passes into the liquid phase and its molar fraction

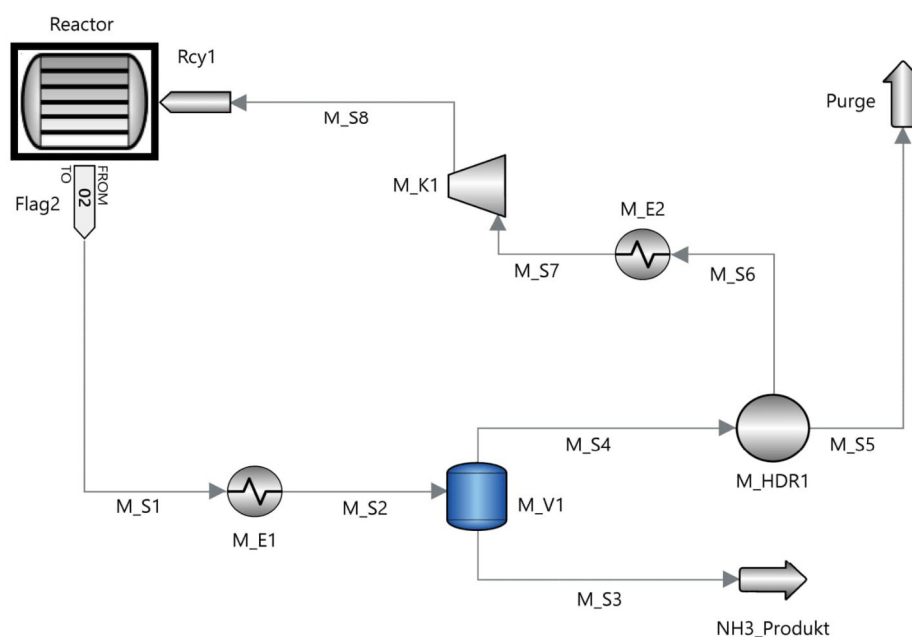


Figure 4. Product condensation and recycling of substrates.

in the vapour phase lowers. This causes the temperature required for condensation to lower as well. Figure 5 shows the Enthalpy – Temperature diagram for mixtures containing 20% (outlet reactor ammonia concentration) of ammonia and stoichiometric ratio of hydrogen and nitrogen.

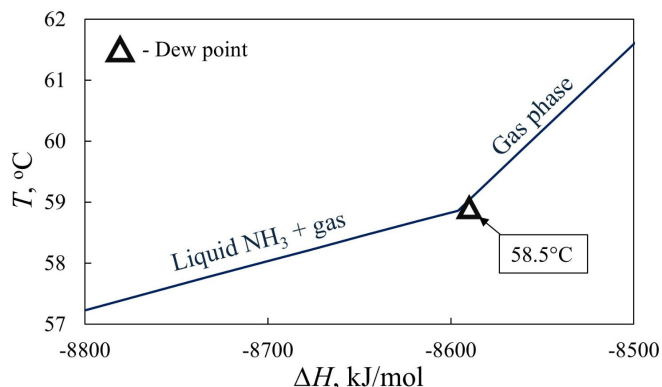


Figure 5. Phase diagram of the mixture with 20% NH_3 in the vapour phase at 200 bar.

An important issue, when it comes to choosing the right condensation conditions is the available cooling media that can be used to lower the system temperature by the required amount. Generally, it is advantageous to use tap water as a cooling medium, as it is widely available and does not need any additional preparation. However this method of cooling is limited with the minimum achievable temperature, which in practice does not go below 20°C . The obtained liquid is separated from the uncondensed gases and is treated as the product of the installation. The purity of the obtained product is kept around 99%.

3.3.2. Recycle

The remaining stream of gases M_S4 is appropriately prepared and then recycled back into the reactor. The preparation process includes splitting the stream into two parts in the M_HDR1 junction: the main recycled stream M_S6 and the purge stream M_S5 , which is discarded to prevent accumulation of unreacted substrates, which unfortunately leads to the unavoidable loss of part of the substrates and product.

The parameter *OutRatio*, expressed by Eq. (13), was defined as the ratio of the purge stream (M_S5) and the recycle stream (M_S4). This parameter was used to control the amount of gases removed from the installation through the purge stream:

$$\text{OutRatio} = \frac{W_{\text{M_S5}}}{W_{\text{M_S4}}} \quad (13)$$

The typical amount of gases discarded into the purge streams oscillates around 1–2% of the primary stream M_S4 . The effect of changing this parameter on our simulation has been

analysed with the use of a case study. It is important to note that the use of a purge stream can be a cause of environmental and safety concerns, as the gases from the installation could be released into the atmosphere and therefore they should be collected, e.g. in additional storage tanks.

After the stream split, the major portion of the gases is then reheated in the heat exchanger M_E2 and recompressed by the compressor M_K1 , to match the parameters of the primary substrate stream flowing into the reactor. Obtaining the right parameters of the recycled gas plays a key role in the functioning of the junction R_HDR1 (see Fig. 3) that introduces the recycled stream back to the reaction section. The pressure and temperature need to be carefully balanced to guarantee the right conditions in the reactor.

4. RESULTS

4.1. Reactor fine-tuning

The considered ammonia synthesis reaction is an exothermic reaction, which causes changes in the temperature distribution within the reactor. This distribution is dependent on the reaction rate on each of the three catalyst beds. Figure 6 shows the temperature gradients over the length of the reactor.

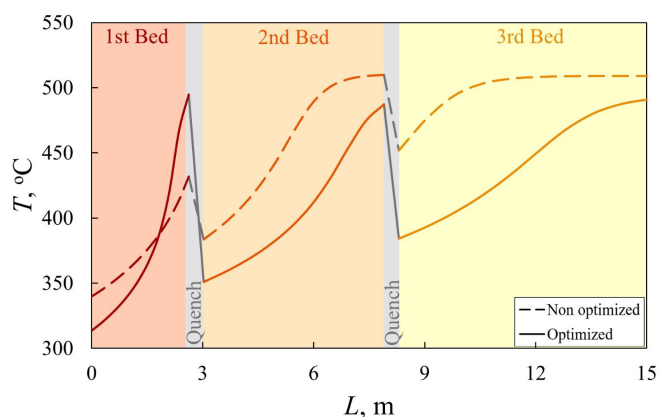


Figure 6. Temperature profile in the reactor for the 23000 kg/h scale.

In order to prevent the decrease of conversion rate while fine-tuning the reactor temperature to keep the catalyst temperature under 500°C , an optimization tool was used. The tool works by changing several specified variables in predefined ranges as well as keeping observed parameters above or below a given value. The changed variables were: the percentage of the feed stream going through the valves XV1-XV4 , controlled by the valve opening degree, as well as the reactor inlet temperature, controlled by the temperature on the junction R_HDR2 . During the process, the molar fraction of ammonia in the stream exiting the reactor has been monitored to prevent the drop of reaction rate.

In Figure 6 temperature profiles for reactor before and after the use of the optimization tool have been shown. The procedure was done for all three scales, the results have been shown in Table 7.

Table 7. Comparison of various scales of ammonia production before and after the use of the optimization tool.

Parameter	23000 kg/h NH ₃		11500 kg/h NH ₃		300 kg/h NH ₃	
	before	after	before	after	before	after
Reactor inlet temperature [°C]	340	313.8	340	309.4	340	309.6
R_XV1 [%]	2.34	11.65	11.90	14.92	32.27	15.11
R_XV2 [%]	30	33.81	30	33.96	30	33.93
R_XV3 [%]	30	46.67	30	47.76	30	47.71
R_XV4 [%]	37.66	7.87	28.10	3.37	7.73	3.25
R_S18 y _{NH₃} [mol. %]	18.71	20.87	19.24	20.94	19.24	20.94

4.2. Premises

To analyse the influence of selected variables on the process performance, a case study method has been utilized. Case study allows for automatic changing of specified variables through a range of values, while simultaneously collecting the data of the observed variables. Table 8 summarises the specified and observed parameters that have been analysed through the case study in the built simulation.

Table 8. Summary of the case study.

Case study	Variable 1	Range	Variable 2	Range	Observed parameters
CS1	M_V1.T	20–45 °C	–	–	W _{NH₃} [kg/h], Q [kJ/kgNH ₃], z _{M_S5} [mol. % NH ₃], W _{M_S5} [kg/h]
CS2	OutRatio	1.2–5.2%	R _{H₂/N₂}	2.8–3.2	W _{NH₃} [kg/h], Q [kJ/kgNH ₃]

4.2.1. Case study 1: Condensation temperature

For the first case study, the impact of changing the condensation temperature was analysed. Temperature ranges (20–45°C) were chosen based on the previously presented H–T phase diagrams (Fig. 5). The case study was done for all three scales. Figure 7 depicts the changes of corrected ammonia stream.

The observed changes of product stream with changing condensation temperature show a clear advantage of using low condensation temperatures. However, the slope of the obtained curve grows as the temperature rises, which might suggest

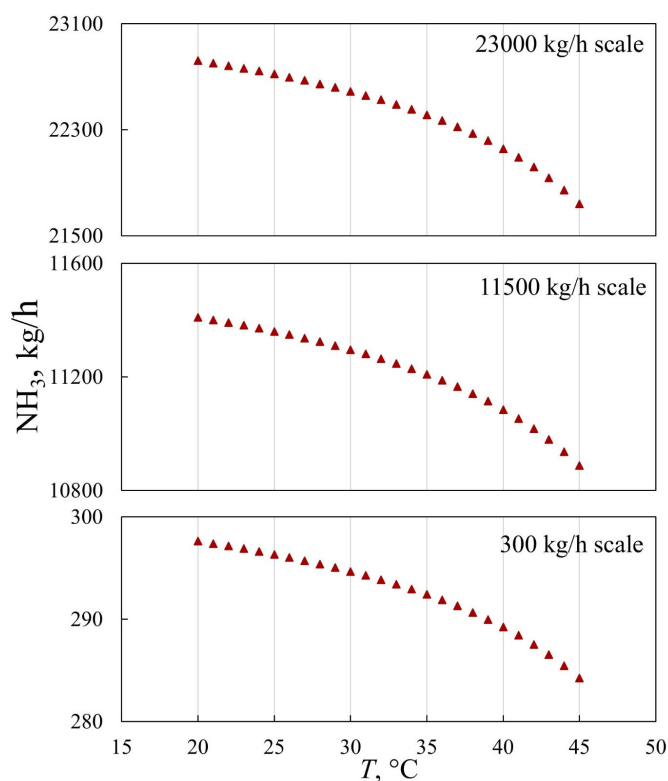


Figure 7. Ammonia flow mass content in the product stream depending on condensation temperature.

a greater tolerance for temperature fluctuations in the lower range of condensation temperatures. Additionally, the case study shows noticeable similarities between the considered scales.

Further analysis has been conducted based on the highest scale of production, as the obtained trends do not differ significantly between the different scales.

Due to the worsening of condensation conditions with growing temperatures, the percentage of leftover ammonia in the vapour phase grows. With the presence of the purge stream, this leads to a higher amount of product loss. Figure 8 depicts the changes in the aforementioned parameters depending on the condensation temperatures.

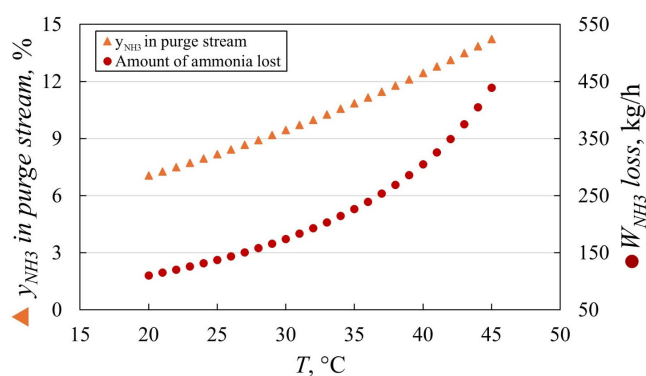


Figure 8. Changes in % of ammonia in the purge stream and loss of product depending on condensation temperature.

The impact of condensation temperature on the energetic requirement of production was analysed next. Figure 9 shows different types of energy demanded by the process per kilogram of produced ammonia: electricity, the heating energy and the cooling energy. Electricity is the energy powering the compressors which increase the pressure of the gases to the desired amount. It is calculated as the sum of the energy usage of all four compressors used in the process. The heating energy is the energy delivered into the system in the heat exchangers heating the gas mixture. It is only used to heat the recycle stream after the condensation step. The cooling energy is the energy taken from the system in the heat exchangers cooling the gas mixture. The heat is taken away by the cooling medium – water. It is used in the substrate preparation step to prevent the temperature of hydrogen from rising too high after its compression, and also in the condensation step, to allow for the separation of the product from the unreacted gases.

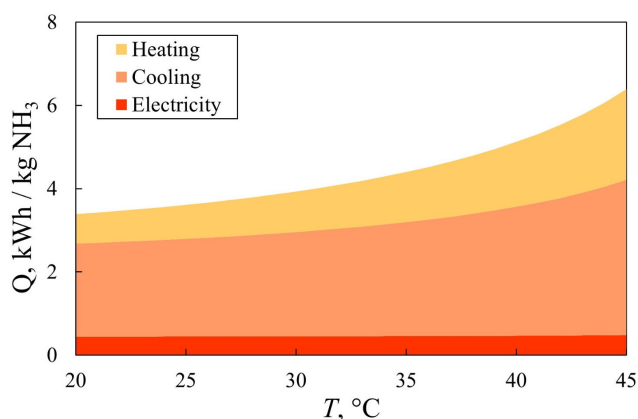


Figure 9. Energy per 1 kg of ammonia produced depending on the condensation temperature.

Based on Figure 9 it can be concluded that lowering the condensation temperature is advantageous from both the production as well as the energetic cost perspective. Both the sum of cooling and heating energies grow with the increase of condensation temperatures. The temperature of 20 °C seems to be the optimal choice, as it improves the efficiency of the process without the need for more expensive cooling media, as it can be achieved by using water as a cooling medium.

4.2.2. Case study 2: Substrate ratio and purge

The following case study shows the impact of changes in the fraction of the purge stream removed from the installation and the ratio of H₂ to N₂ (R_{H_2/N_2}).

The first observed parameter was the ammonia stream. Figure 10 depicts the changes in ammonia stream for the largest scale.

Figure 10 shows clear improvement of ammonia production with lower *OutRatio* and ratio of the substrates around 3. The differences between the results for lowest and highest values of *OutRatio* are quite significant, losing over 2000 kg/h of product. However, the stoichiometry seems to have a lesser impact on the product stream, as even the values for the highest and lowest examined ratios of 3.2 and 2.8 show less than 800 kg/h difference from the highest obtained production at the ratio of 3.

The impact of the change of the studied variables has also been analysed in the context of changing energy requirements per 1 kg of produced ammonia. Figures 11 with 12 show a total of four heatmaps, demonstrating the influence of changing *OutRatio* and stoichiometry on the sum of energy used per 1 kg of ammonia as well as the changes of three types of energy: cooling, heating and electric energy. The total energy, as well as the cooling and heating energy show similar trends, as for all of them, the stoichiometric ratio of 3 shows a clear value decrease. What can also be observed, is that with the increasing *OutRatio*, the results for different stoichiometric ratios seem to be closer in value, which is demonstrated on the heatmaps with a smoother colour gradient. However, when considering the electrical energy used for the compression of the gases, the trend varies significantly from the previous examples, as the energy per 1 kg of ammonia quickly rises with the increase of *OutRatio*, for all considered stoichiometries. However, the electricity used in the process constitutes only a small percentage of the total energy and that is why its influence on the total energy trends is negligible.

4.2.3. Process energy requirement and energy density

In this study, ammonia is treated as an energy carrier in which the energy supplied during the synthesis process is stored in the form of chemical energy. The cumulative enthalpy demand along the entire process pathway, including compression and heat exchange, constitutes a measure of the energy input required to produce this carrier. This approach is complementary to the definition of energy density based on the lower heating value of ammonia, which describes the maximum amount of energy that can be recovered during combustion. Considering both perspectives enables a coherent thermodynamic assessment of ammonia as an energy carrier.

In order to show the thermodynamic impact of the process, changes of the enthalpies of substrates and product streams were analysed, which were the stream enthalpy values (ΔH), molar flow rates (F) and enthalpy streams rate ($\dot{H}$).

Table 9 presents exemplary data for the lowest scale of ammonia production. The domination of negative enthalpy streams in the process is caused by the exothermic nature of the reaction and the heat delivered by the product stream during the condensation step. Due to this, the process, in a thermodynamic sense, leads to the release of energy from the system,

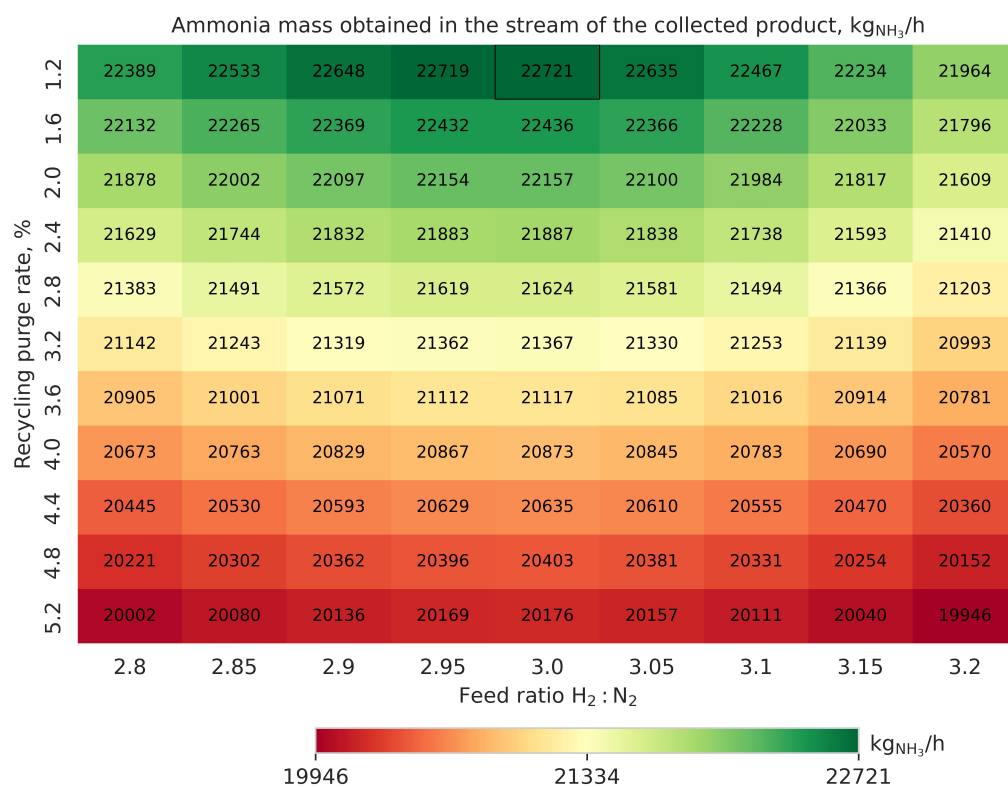


Figure 10. Heat map of ammonia flow mass content in the product stream of the biggest production scale.

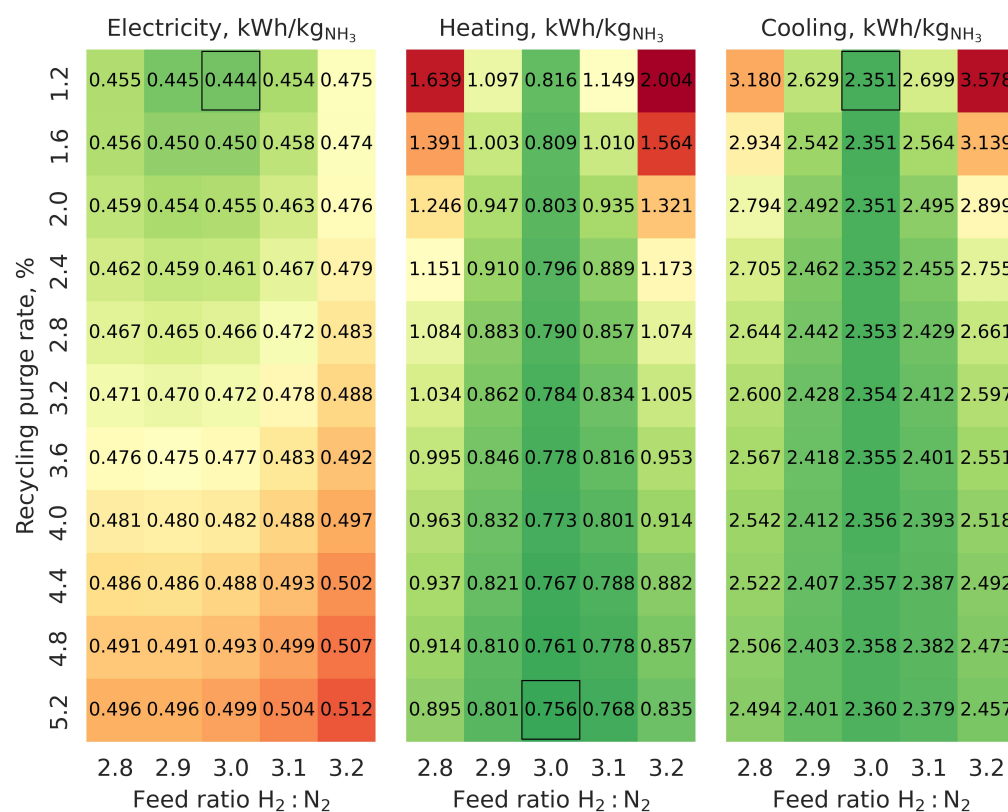


Figure 11. Heat maps of kWh of energy per 1kg of produced ammonia, broken down by energy type: electricity, heating, cooling.

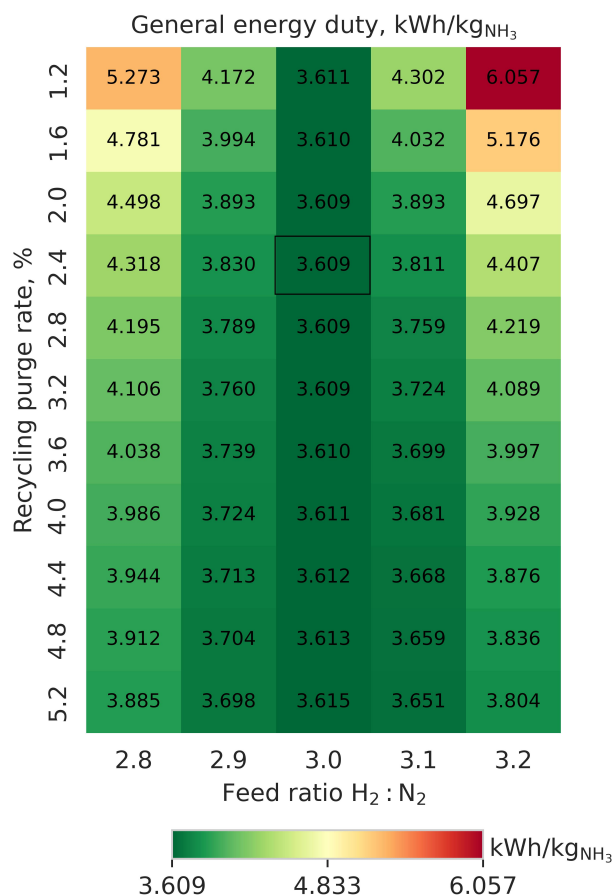


Figure 12. Heat map of kWh of total energy per 1kg of produced ammonia, the result of aggregating the constituent types of energy: electricity, heating and cooling.

Table 9. Enthalpy data of the input and output streams of the process for the lowest scale of ammonia production.

Stream	ΔH [kJ/kmol]	F [kmol/h]	$\hat{H}$ [kJ/h]
S_H ₂	1603	27.5	44045
S_N ₂	-5686	9.2	-52065
NH ₃ _Product	-65831	17.7	-1166583
Purge	-3857	1.3	-4997

which has both positive and negative consequences. Although the exothermic nature of the process allows for lower energy consumption of the installation, it can negatively influence the energy density of the produced product, as some of the chemical energy of hydrogen is released during the synthesis process.

The process energy requirement as part of energy density of the system was analysed in more detail, as it has been split into three categories: the duty of the heating of heat exchangers, the duty of the cooling of heat exchangers and the electricity power of the compressors. In order to avoid cancellation of the signs, all of the values have been summed up as an absolute value, avoiding the negative sign. Table 10 and Figure 13 demonstrate the energy consumption of the system.

Table 10. Summary of process energy requirement.

Scale	Electricity [kW]	Cooling [kW]	Heating [kW]	Sum [kW]
23000 kg/h NH ₃	10092.7	53447.8	18573.8	82114.3
11500 kg/h NH ₃	5030.5	26654.7	9234.1	40919.2
300 kg/h NH ₃	130.9	695.2	241.1	1067.2

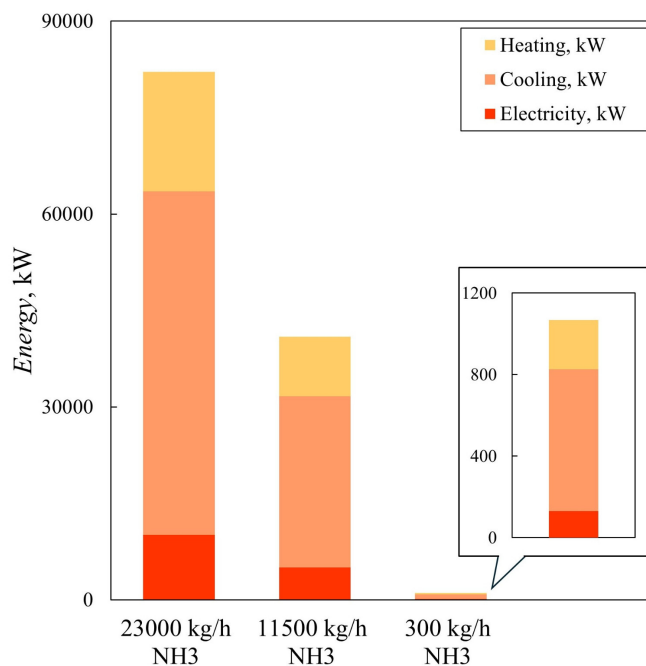


Figure 13. Heating, cooling and electricity demands for three scales of production.

Figure 13 shows clear domination of cooling energy as the biggest part of the total energy consumed by the process. This is caused by the need to vastly lower the temperature of the outlet reactor mixture in order to separate ammonia from the unreacted gases. The temperatures analysed through the case study (20–45°C) are temperatures achievable with using water as a cooling medium. In the prepared simulation, cooling energy was lowered by implementing the quench cooling, which cools the reaction mixture by mixing a cooler stream of gases with the hot stream exiting the catalytic bed.

Compared to the cooling energy, heating energy and electricity used for compression are relatively low. That is because the considered reaction is exothermic, which allows for the heating of the substrates by the outlet reactor mixture. The gases are also heated through the compression process. In order to further minimize the demand of heating energy, a more complex system could be considered, which recycles the heat taken from the cooling of the product in the condensation step.

In the presented analysis, compressor power demand was calculated based on idealized compression work. To better reflect realistic operating conditions at the pre-design stage, addi-

tional losses associated with non-ideal compression behaviour were considered. An isentropic efficiency of 75% which was assumed for all compressors and that of 80% for heat exchangers are conservative engineering assumptions. Furthermore, the model accounts for heat exchangers to ensure realistic thermal management across the system. These efficiency values were kept constant across all investigated production scales. The impact of these assumptions was analysed for all three production scales (i.e. 300, 11 500 and 23 000 kg/h NH_3), and the resulting compressor efficiencies and effective electrical energy consumption are summarized in Tables 11–12.

Table 11. Compressor and heat exchanger efficiency.

Parameter	Efficiency [%]
Compressor Isentropic efficiency	75
Heat Exchanger efficiency	80

Table 12. Compressor and heat exchanger efficiency.

Equipment type	Equipment ID	Power/heat duty [kW]		
		300 kg/h NH_3	11500 kg/h NH_3	23000 kg/h NH_3
Compressor	S_K1	3	125	250
	S_K2	68	2599	5199
	S_K3	59	2256	4513
	M_K4	1	51	131
Heat exchanger	M_E1	−459	−17590	−35272
	M_E2	241	9234	18574
	S_E1	−63	−2416	−4833
	M_V1	−173	−6649	−13343

Ammonia synthesis has been considered as a method of increasing the energy density of hydrogen produced through environmentally friendly methods. This approach solves the problems concerning the problematic storage conditions of hydrogen. In the simulation, energy densities of substances have been defined for the source stream of hydrogen and the process product with Eqs. (14)–(17), respectively:

$$\text{Energy Density}_{\text{H}_2} = \text{LHV}_{\text{H}_2} \cdot \rho_{\text{H}_2} \quad (14)$$

$$\text{Energy Density}_{\text{H}_2\text{KG}} = \text{LHV}_{\text{H}_2} \quad (15)$$

$$\text{Energy Density}_{\text{NH}_3} = \text{LHV}_{\text{NH}_3} \cdot \rho_{\text{NH}_3} \quad (16)$$

$$\text{Energy Density}_{\text{NH}_3\text{KG}} = \text{LHV}_{\text{NH}_3} \quad (17)$$

The described parameters were used to evaluate changes in the suitability of hydrogen and ammonia as energy carriers for storage and transport, by defining energy density in a two-way approach: a mass basis, as Lower Heating Value (LHV), described with Eq. (15) and Eq. (17), with a unit of MJ/kg, and a volume basis described with Eq. (14) and Eq. (16), with a unit of MJ/m³.

In order to better visualize the change in the parameters, the following ratios were defined with Eqs. (18)–(19):

$$\text{Energy Density Ratio} = \frac{\text{Energy Density}_{\text{NH}_3}}{\text{Energy Density}_{\text{H}_2}} \quad (18)$$

$$\text{Energy Density Ratio}_{\text{KG}} = \frac{\text{Energy Density}_{\text{NH}_3\text{KG}}}{\text{Energy Density}_{\text{H}_2\text{KG}}} \quad (19)$$

The calculated values are shown in Table 13.

Table 13. Change in LHV based energy density.

Hydrogen energy density ¹ [MJ/m ³]	Hydrogen energy density [MJ/kg]	Product energy density [MJ/m ³]	Product energy density ² [MJ/kg]	Energy Density Ratio	Energy Density Ratio KG
72.9	119.9	11402	18.6	156	0.16

¹ Energy density per 1 m³ of hydrogen at 80 °C and 8.9 bar.

² Energy density per 1 m³ of ammonia at 25 °C and 200 bar.

The data shown in Table 13 demonstrate how the ammonia synthesis process affects the energy density of the system. There is a considerable increase in the energy per volume, showing the improvement of storage and transport efficiency when ammonia is used as an energy carrier, as it allows more amount of energy to be kept in a smaller volume. However, a noticeable trade-off appears to be the energy density considered in the context of mass, as 1 kg of ammonia is able to deliver less energy than 1 kg of hydrogen. The impact of the hydrogen conversion to ammonia on the energy density of the system is shown in Figure 14.

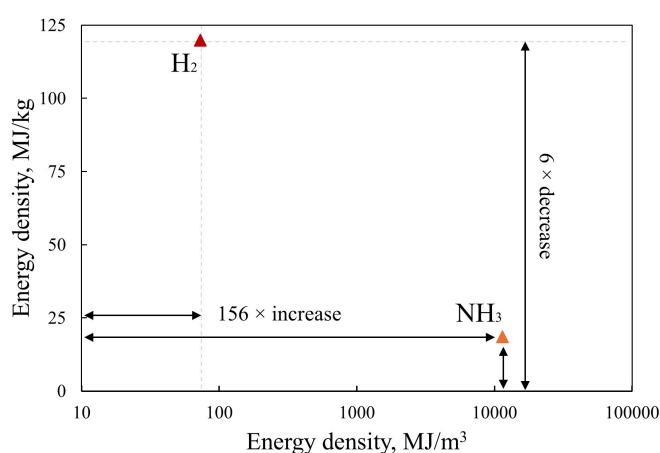


Figure 14. Obtained changes of energy density.

5. CONCLUSIONS

Based on the results presented in this work it can be concluded that the presented process is a promising solution for increasing the energy density of hydrogen, which in light

of current attempts aimed at promoting renewable energy sources as feasible alternatives to fossil fuels, stands as an important area of development. The created simulation operates within the range of optimal conditions sufficient at the pre-engineering stage and demonstrates high numerical stability allowing it to be subjected to numerous experiments and further tuning for the needs of a specific application.

The proposed solution has been analysed from production efficiency and energetic cost perspectives, which show the importance of selecting the proper process conditions to balance the energy consumption with maximum amount of obtainable product. The analysis of the different types of energy used in the process allows for a better understanding of the possible improvements to the process, which help with implementing solutions of circular economy. The study also contributes to the development of the research area related to the conversion of hydrogen to ammonia by presenting the impacts of possible divergence from stoichiometric ratio of reagents, which are common in the industry.

From the industrial perspective, the developed installation demonstrates the potential for effectively utilizing ammonia synthesis process as a potential method for hydrogen storage in a form with higher energy density, ensuring safer conditions. This technology is applicable not only in large-scale industrial installations but also in smaller, decentralized energy systems.

ACKNOWLEDGEMENTS

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SYMBOLS

a	constant in the SRKM model
A	pre-exponential factor, $\text{mol}/(\text{s} \cdot \text{m}^3 \cdot \text{atm}^{1.5})$, $\text{mol} \cdot \text{atm}^{0.5}/(\text{s} \cdot \text{m}^3)$
b	constant in the SRKM model
D	reactor diameter, m
d_{cat}	catalyst particle diameter for Ergun pressure drop correlation, mm
DP	reactor pressure drop, Pa
DP_{elem}	pressure drop per reactor element, Pa
E	activation energy, J/mol
F	molar flowrate, kmol/h
ΔH	enthalpy, kJ/mol
$\hat{H}$	enthalpy stream, kJ/h
k	reaction rate constant, $\text{mol}/(\text{s} \cdot \text{m}^3 \cdot \text{atm}^{1.5})$, $\text{mol} \cdot \text{atm}^{0.5}/(\text{s} \cdot \text{m}^3)$
L	reactor length, m
L_{elem}	reactor element length, m

MW	molecular weight, kg/kmol
N_e	number of segments used in the Reactor, –
p	pressure, bar, kPa
Q	energy consumption per 1 kg of ammonia, kWh/kg
R	gas constant, J/(mol · K)
r	reaction rate, kmol/(s · m ³)
$R_{\text{H}_2/\text{N}_2}$	molar feed ratio of hydrogen to nitrogen, –
T	temperature, °C
v	velocity of fluid in tubes, m/s
V	volume, m ³
W	mass flow rate, kg/h
x	molar fraction in the liquid phase, mol/mol
y	molar fraction in the gas phase, mol/mol
z	molar fraction in the gas and liquid phase, mol/mol

Greek symbols

ε	void fraction, m ³ /m ³
μ	viscosity, Pa · s
ρ	mass density, kg/L

Subscripts

1, 2	number of component
NH ₃ , H ₂ , N ₂	compound type
p	packing density
o	operational

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