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SUSTAINABLE ENERGY

Exploring the Potential of Ammonia/Hydrogen Trigeneration Cycle

Numerous low-carbon energy initiatives are adopting ammonia as an energy source, with a particular focus on combining ammonia and hydrogen in a 70%/30% volume ratio for gas turbine systems. The ammonia-hydrogen triple generation cycle, a hybrid of a humidified Brayton cycle and a reverse Brayton cycle, has demonstrated outstanding performance, achieving zero carbon and low NOx emissions, while boosting overall efficiency to around 59%, comparable to conventional fossil fuel-based power generation systems. The Aspen Plus software was used to simulate and calculate the system's efficiency, mainly focusing on the humidification Brayton cycle, reverse Brayton cycle, and waste heat recovery phase of the ammonia-hydrogen triplex production cycle. Three scenarios were developed to evaluate the efficiency of different steam condensation recovery processes, with all three yielding efficiencies of at least 59%, confirming the cycle's effectiveness and feasibility. Advancements in the system's structure in the future could further enhance the system's efficiency.

Keywords:
Gas turbine, ammonia combustion, thermodynamic cycles, aspen plus, waste heat recovery.

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INTRODUCTION

The world today is facing unprecedented needs to meet energy demand while reducing energy costs and pollution levels. Fossil fuels, which have been the dominant energy source for decades, are becoming increasingly scarce and expensive to extract, posing a significant challenge to meeting this growing demand. This has prompted a shift towards renewable energy sources such as solar, wind, and hydropower, and alternative energy fuels like ammonia and hydrogen, which are sustainable and emit fewer pollutants. In this paper, we present the progress that has been so far in evaluating the performance of our previously proposed ammonia-hydrogen trigeneration power cycle [1, 2]. The thermodynamic cycle, including its three different scenarios, was processed and simulated using Aspen Plus Software. Efficiency calculations were subsequently performed using the resulting data.

SIMULATION METHODS

The ASPEN Plus software, an advanced system for process engineering, is used to model and simulate thermodynamic engineering cycles. It has been extensively used and its ability to simulate real-world power plant applications has been proven and demonstrated in many research articles [3-5].

Three different scenarios were utilised to simulate the trigeneration cycles. In each scenario, the water vapour from the combustion gases was separated by cooling at different stages within the system. These included i) the separation of the water stream from the exhaust gases behind the first heat exchanger (Scenario 1, Fig. 1), ii) the separation of the water stream from the exhaust gases behind the second heat exchanger (Scenario 2, Fig. 2), and iii) the complete absence of condensate (Scenario 3, Fig. 3 overleaf).

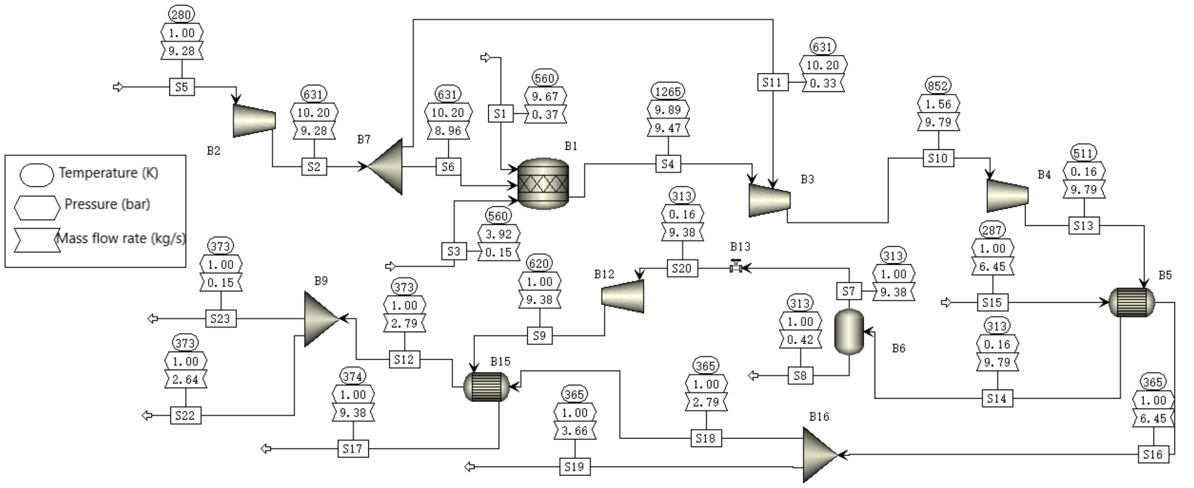

Fig. 1. Scenario 1: separation of water stream from the exhaust gases behind the first heat exchanger.

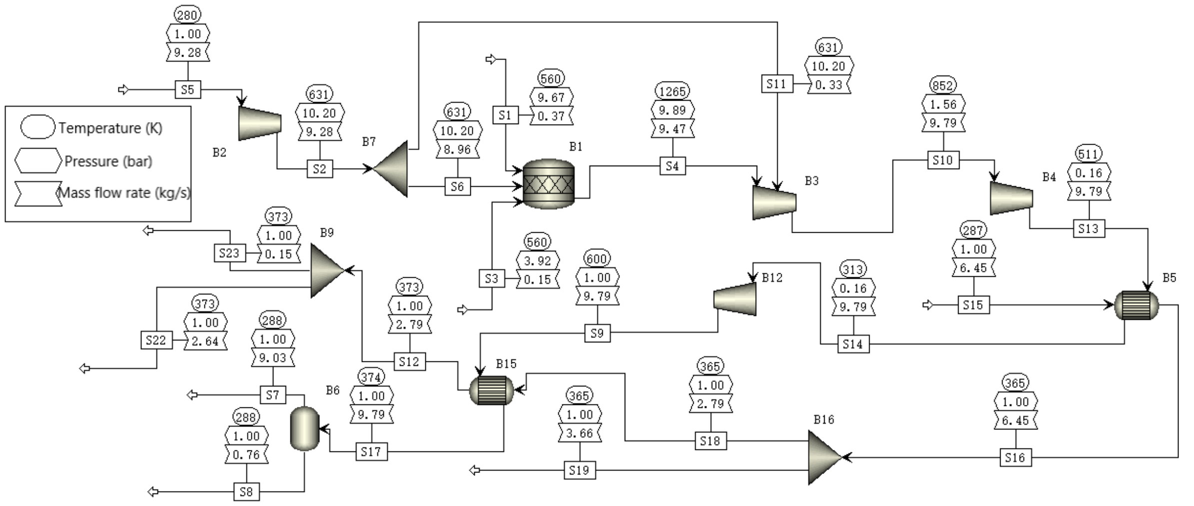

Fig. 2. Scenario 2: separation of water stream from the exhaust gases behind the second heat exchanger.

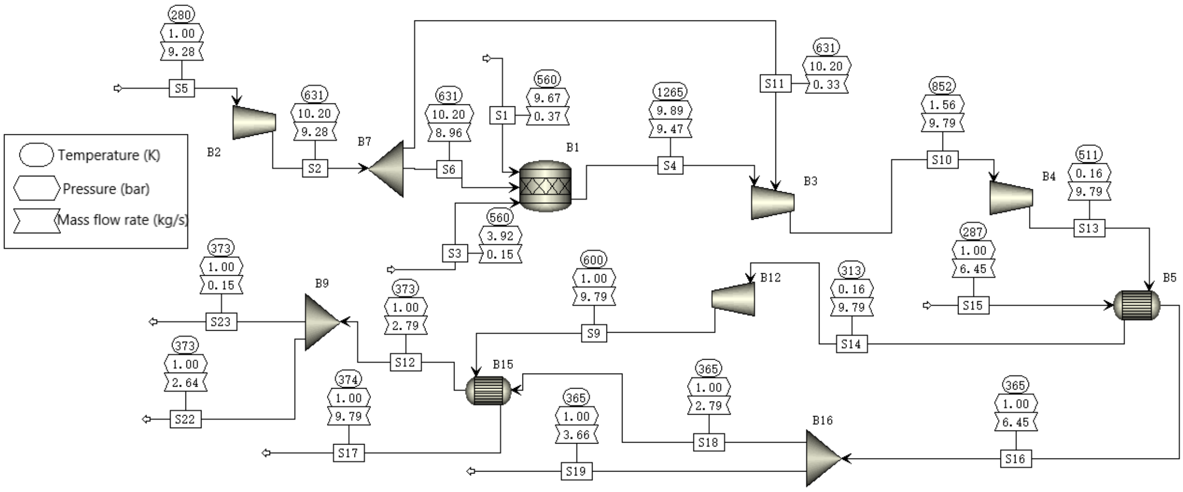

Fig. 3. Scenario 3: no water was separated.

Initially, the incoming atmospheric air (with a mass flow rate of 9.28 kg/s, temperature of 280K and pressure of 1.00 bar) was compressed by the compressor (B2). Subsequently, the compressed air was split into two distinct streams with different amounts of $\dot{m}$ via a splitter (B7). One of the streams was directed to the gas turbine (B3) to facilitate the cooling of its blades, while the second stream was fed into a combustion chamber (B1) to undergo combustion with an NH3-H2 mixture by 70%/30% (vol.%). In order to reduce the production of nitrogen oxides, water vapour was added to the combustion chamber (B1). The chemical reaction inside the combustion chamber can be given as:

$$0.7NH_3 + 0.3H_2 + 0.675O_2 \rightarrow 0.35N_2 + 1.35H_2O$$

The flue gases resulting from the combustion process were expanded by both the first gas turbine (B3) and the second gas turbine (B4), respectively. It is to be noted that the exhaust gases from the second gas turbine (B4) were found to still contain a significant amount of heat, which could be harnessed to heat water and ultimately increase the thermal efficiency of the system. Consequently, the turbine's exhaust gasses are directed towards the first heat exchanger (B5) to elevate the temperature of the liquid water from 287K to 365K, while the exhaust gases were cooled to 313 K. A splitter (B16) was employed to divide the resulting hot water into two streams with varying mass flow rates. One of the streams was utilised for dynamic district heating, while the second stream was heated using the second heat exchanger (B15). The resulting water flow was then divided into two streams using splitter (B9), with one having a mass flow rate of 2.64 kg/s intended for industrial heating, and the other having a mass flow rate of 0.147 kg/s, which was heated to 560 K and directed back to the combustion chamber for the subsequent triple generation cycle. Once the exhaust gases had passed through the first heat exchanger (B5), the variations among the three simulation scenarios would become apparent.

In the first simulation scenario (Fig. 1), the exhaust gases that passed through the first heat exchanger were directed to the separator. Here, a portion of the water vapor present in the exhaust gases underwent condensation, resulting in the formation of a liquid under standard atmospheric pressure and was then separated in accordance with the two-phase flow. The recovered liquid water was utilised as part of the feed water for the waste heat recovery process after passing through separator (B6). The residual gases were then passed through the expansion valve (B13), followed by compression in compressor (B12). This sequence of processes led to an increase in the gases' temperature to 620K at 1.00 bar. Finally, the exhaust gases were cooled to 374K in the second heat exchanger (B15), utilising a water stream with a temperature of 365K, and subsequently released.

In the second scenario (Fig. 2), the exhaust gases exited the first heat exchanger (B5) at 313K and 0.16 bar was fed directly into the second compressor (B12). The pressurised gas was then directed into the second heat exchanger (B15), where it underwent a heat exchange process with the supply water. Within separator (B6), the exhaust gases were completely cooled down to 288K, with the majority of the water vapour undergoing cooling and condensation into liquid water. The resulting liquid water, with a mass flow rate of 0.76 kg/s, was subsequently retrieved in a subsequent stage as part of the supply water for heating work, while the remaining exhaust gases were discharged.

The final simulation scenario (Fig. 3) involved no separation of water from the exhaust gases. Once the exhaust gases exited the first heat exchanger (B5), it was directly routed into the second compressor (B12), without undergoing any treatment. The exhaust gases at 0.16 bar were then compressed to 1.00 bar, which was the same as in the second scenario. Subsequently, the exhaust gases underwent a heat exchange (B15) with the supplied liquid water from the second splitter (B16). Following this step, the exhaust gases were directed to the subsequent processes.

RESULTS AND DISCUSSION

The present study involves an evaluation of the performance of a trigeneration thermodynamic cycle through three different simulation scenarios. The overall efficiency was determined by taking into account various parameters, such as the thermal power supplied by fuel combustion, the mechanical efficiency and work output of the gas turbines, and the power consumed by the compressors.

In the first scenario, a mass flow rate of 0.42 kg/s was utilised to condense and separate water, leading to a computation of a water circulation efficiency of 6.51%. In terms of the first heat exchanger (B5), 2.14 MW of heat was released from the gas, and an enthalpy change of 2.11 MW was achieved for the heated water, resulting in an efficiency of 98.35%. Similarly, in the second heat exchanger (B15), approximately 2.51 MW of heat was released from the gas, and an enthalpy change of 2.10 MW was attained for the warmed water, which led to an efficiency of 82.21%. The input thermal power provided 1.07 MW to the system, the two gas turbines (B3 and B4) delivered a total of 7.12 MW with 90% mechanical efficiency, and the two compressors (B2 and B12) consumed a total of 6.47 MW of power. This resulted in an overall system efficiency of 60.69% and recovery of 0.42 kg/s of water.

In the second scenario, the efficiency of the first heat exchanger (B5) was found to be the same as in the first scenario, at 98.35%, owing to their identical processes. Nonetheless, other differences emerged in the efficiency calculations between the two scenarios. The mass flow rate of the condensate in scenario 2 was 0.76 kg/s, producing a water circulation efficiency of 11.78%. The second heat exchanger (B15) in scenario 2 released approximately 2.48 MW of heat during combustion and cooling, and the enthalpy change of the water during heating was 2.02 MW, leading to an efficiency of 81.71%. The simulation revealed that the input thermal power provided 1.07 MW to the system, and the gas turbines (B3 and B4) delivered a total of approximately 7.12 MW with a mechanical efficiency of 90%. The total power required to operate the two compressors (B2 and B12) was approximately 6.49 MW. Consequently, the system's overall efficiency was found to be 59.04% with 0.76 kg/s of recovered water.

In the third scenario, the sole distinction from Scenario 2 is the absence of water vapor condensation and separation in the exhaust gas downstream of the second heat exchanger (B15). Therefore, with the exception of the water circulation efficiency, all other efficiencies in Scenario 3, namely the first heat exchanger (B5) efficiency, the second heat exchanger (B15) efficiency, and the system efficiency, are in agreement with the calculations in Scenario 2. As the mass flow rate of the condensate is zero in Scenario 3, the water circulation efficiency is also zero. The efficiency of the system in Scenario 3 closely approximates that of Scenario 2, at 59.04% without any water recovered from the system.

CONCLUSIONS

The present study aimed to investigate the feasibility of an ammonia-hydrogen trigeneration cycle, which integrates a humidified Brayton cycle and a reverse Brayton cycle, as a competitive and promising option for ammonia-based energy utilisation in the contemporary energy market. The system's efficiency was analyzed using Aspen Plus software under various scenarios, followed by validation and efficiency calculations.

The simulation results demonstrated that the efficiency of the system, heat exchanger efficiency, compressor power consumption during waste heat recovery, and water circulation efficiency were significantly affected by the water condensation and recovery at different stages. The first scenario exhibited a lower water circulation efficiency of 6.51% compared to the second scenario, which achieved an efficiency of 11.78%, due to the differences in the condensation methods employed at different stages in the two scenarios. However, the second heat exchanger in Scenario 1 exhibited the highest efficiency of 82.21% among the three scenarios. In contrast, the third scenario showed a 0% water circulation efficiency due to the absence of water condensation and separation in the system. Nevertheless, all other efficiencies in Scenario 3 were consistent with those in Scenario 2. Moreover, the overall system efficiencies remained at approximately 59%, despite the variations in water condensation and recovery at different stages. Among the three scenarios, Scenario 1 achieved the highest system efficiency of 60.69% by performing water condensation and separation after the first heat exchanger.

In conclusion, the study found that condensing and separating water vapour between the first heat exchanger and the second compressor in the ammonia-hydrogen trigeneration cycle system is the most effective way to improve the system's efficiency, even though it may not be the most efficient water cycle in the simulation. However, this can be improved by adding another separator after the second heat exchanger. The simulation results also confirmed the feasibility and high efficiency of the ammonia-hydrogen trigeneration cycle, which can compete with current fossil fuel-based power generation systems. The study suggests that with further technological development, the ammonia-hydrogen trigeneration cycle can become even more efficient and play a significant role in the low-carbon energy structure. Nevertheless, there is an immediate need to evaluate the exhaust gas emission levels of the cycle across the three scenarios.

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Conflicts of interest
The authors declare no conflict of interest.

REFERENCES

[1] M. Guteša Božo, S. Mashruk, S. Zitouni, and A. Valera-Medina, 'Humidified ammonia/hydrogen RQL combustion in a trigeneration gas turbine cycle', *Energy Conversion and Management*, vol. 227, p. 113625, Jan. 2021. doi.org/10.1016/j.enconman.2020.113625

[2] M. Guteša Božo e*t al.*, 'A novel trigeneration gas turbine cycle powered by humidified ammonia/hydrogen with ammonia refrigeration', presented at *1st Symposium on Ammonia Energy*, 2022.

[3] Ö. Ç. Mutlu and T. Zeng, 'Challenges and Opportunities of Modeling Biomass Gasification in Aspen Plus: A Review', *Chem. Eng. & Technol.*, vol. 43, no. 9, pp. 1674–1689, Sep. 2020. doi.org/10.1002/ceat.202000068

[4] M. Garcia, H. K. Knuutila, and S. Gu, 'ASPEN PLUS simulation model for CO 2 removal with MEA: Validation of desorption model with experimental data', *Journal of Environmental Chemical Engineering*, vol. 5, no. 5, pp. 4693–4701, Oct. 2017. doi.org/10.1016/j.jece.2017.08.024

[5] C. Panda, 'ASPEN PLUS simulation and experimental studies on biomass gasification', B Tech thesis, National Institute of Technology, Rourkela, India, 2012.

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