

# Development and Simulation of Capture and Utilization System for NO<sub>x</sub> Gas from NH<sub>3</sub> Combustion

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Ammonia (NH<sub>3</sub>) combustion is gaining increasing attention as a zero-carbon fuel due to its advantages in production, storage, and transportation. However, several challenges—such as its low flammability and the risk of nitrogen oxide (NO<sub>x</sub>) emissions—must be addressed before NH<sub>3</sub> can be widely implemented in energy systems. To overcome the NO<sub>x</sub> emission challenge of NH<sub>3</sub> combustion, this study focuses on the development and evaluation of a NO<sub>x</sub> capture and utilization system. As a case study of NO<sub>x</sub> utilization, potassium nitrate synthesis via alkaline absorption using potassium hydroxide was selected. A simulation-based analysis was conducted for an NH<sub>3</sub>-fired combined-cycle power plant integrated with the proposed system. The system's value was assessed based on the combined outputs of electricity and the chemical product. The simulation results demonstrated that utilizing NO<sub>x</sub> at an equivalence ratio (ER) of 0.5 can increase total profit by 53 % compared to low-NO<sub>x</sub> combustion at an ER of 1.1. These findings highlight the high feasibility of the proposed system as a chemical recycling approach and underscore its significant potential for future development.

## 1. Introduction

The combustion and utilization of fossil fuels have long provided cheap and abundant energy sources for the development of human society. However, the large-scale emission of pollutants and greenhouse gases from the power sector has led to serious anthropogenic hazards and critical climate change. Governments and organizations worldwide have implemented various countermeasures to mitigate the environmental impact of such human activities. Toxic and hazardous pollutants—such as sulfur oxides (SO<sub>x</sub>) and nitrogen oxides (NO<sub>x</sub>)—are strictly regulated. At the same time, emissions of greenhouse gases, particularly carbon dioxide (CO<sub>2</sub>), are receiving increasing attention and regulation due to the escalating threat of global warming.

Current decarbonization strategies for the power sector include the replacement of thermal power with renewable energy sources, the substitution of fossil fuels with decarbonized alternatives, improvements in power generation efficiency, and the deployment of carbon capture, utilization, and storage (CCUS) technologies (Rahimi et al., 2024). Among these strategies, the complete or partial replacement of combustion fuels with decarbonized alternatives, including carbon-neutral and zero-carbon fuels, is regarded as a mid-term transformation approach for existing thermal power plants (Nose et al., 2023). Moreover, such fuels offer the potential for large-scale carbon-free energy storage and conversion in a future decarbonized society.

In recent years, ammonia (NH<sub>3</sub>) has attracted growing attention as a promising zero-carbon fuel (Gao et al., 2017). Unlike hydrogen gas, NH<sub>3</sub> has a higher boiling point, enabling easier storage and transportation under lower pressure and higher temperature conditions. Additionally, the industrial-scale production of NH<sub>3</sub> via the Haber–Bosch process is well-established, making it capable of meeting the increasing demand for mid-term decarbonization in thermal power applications.

Nevertheless, the adoption of NH<sub>3</sub> as a fuel poses several challenges. For instance, its flammability is significantly lower than that of conventional fuels. As a reference, the maximum laminar burning velocity of NH<sub>3</sub> is approximately 8 cm/s, which is only about 23 % that of methane, the slowest among all major hydrocarbon fuel gases (Murai et al., 2019). Another challenge arises from the potential for substantial NO<sub>x</sub> emissions during NH<sub>3</sub> combustion. While conventional fuels produce thermal NO<sub>x</sub> through the oxidation of atmospheric nitrogen at high temperatures, NH<sub>3</sub> combustion produces fuel NO<sub>x</sub> in addition to thermal NO<sub>x</sub> due to the oxidation of

nitrogen present within the fuel itself. This results in elevated  $\text{NO}_x$  concentrations in the exhaust gas of  $\text{NH}_3$  combustion (Murai et al., 2019). Emissions of  $\text{NO}_x$  pose serious environmental and health risks, contributing to respiratory and mucosal diseases and environmental degradation via acid rain formation (Zhu and Xu, 2022). Consequently,  $\text{NO}_x$  emissions are regulated globally through various environmental policies. For example, the Japanese government has enforced the Air Pollution Control Act since 1968, which includes stringent  $\text{NO}_x$  emission limits. These regulations have become increasingly strict in response to societal and technological advancements, aiming to protect the environment and public health.

Therefore, various  $\text{NO}_x$  mitigation technologies have been developed to address the increased  $\text{NO}_x$  emissions from  $\text{NH}_3$  combustion. These include reducing  $\text{NO}_x$  formation through partial decomposition of  $\text{NH}_3$  (Nose et al., 2023), optimizing combustion conditions (Skryja et al., 2014), and post-combustion removal technologies. Among these, Selective Catalytic Reduction (SCR) is a widely adopted and commercialized post-combustion de- $\text{NO}_x$  technology in Japan (Ministry of the Environment(Japan), 2014). SCR employs selective reductants such as  $\text{NH}_3$  and specific catalysts to convert  $\text{NO}_x$  into nitrogen and water. However, although SCR is simple, stable, and highly efficient, it involves operational costs related to the consumption of reductants and energy, as well as catalyst degradation. These costs become particularly significant when applied to  $\text{NH}_3$  combustion, which inherently generates more  $\text{NO}_x$ . As a result, current studies focus on developing low- $\text{NO}_x$   $\text{NH}_3$  combustion technologies to reduce the need for post-combustion treatment. However, this often comes at the cost of reduced power generation efficiency per unit of  $\text{NH}_3$  used.

On the other hand, since  $\text{NO}_x$  is the dominant acidic component in the exhaust gas from  $\text{NH}_3$  combustion, the  $\text{NO}_x$  selectivity character of SCR may not be essential. Moreover, considering that  $\text{NO}_x$  is a raw material in nitric acid production, the dilute but relatively pure  $\text{NO}_x$ -containing exhaust gas from  $\text{NH}_3$  combustion presents a promising opportunity for value-added utilization rather than mere pollutant treatment. By harnessing the reactivity of  $\text{NO}_x$  through appropriate chemical pathways, it is possible to achieve environmental protection and resource recovery simultaneously. Nevertheless, few studies have explored the direct utilization of emitted  $\text{NO}_x$  for valuable material production, leaving its feasibility largely uncertain.

## 2. Proposed System

To address the existing uncertainty regarding  $\text{NO}_x$  treatment through valuable material production, the authors proposed a novel  $\text{NO}_x$  capture and utilization system that treats  $\text{NO}_x$ -containing exhaust gas as a raw material for producing value-added products. The goal is to offset or surpass the costs associated with conventional  $\text{NO}_x$  treatment through the economic value of the generated products. To evaluate the feasibility of this concept, the present study conducted a preliminary techno-economic analysis of an  $\text{NH}_3$ -fired combined-cycle power plant integrated with the proposed  $\text{NO}_x$  capture and utilization system.

In this study, a system was proposed to harness the chemical reactivity of  $\text{NO}_x$  to produce the value-added material with market potential. Potassium nitrate ( $\text{KNO}_3$ ) was selected as the target among various possible products due to its commercial value as a chemical fertilizer and raw material in gunpowder production. The system employed an alkaline absorption method, using potassium hydroxide ( $\text{KOH}$ ) as the absorbent to capture  $\text{NO}_x$  and synthesize  $\text{KNO}_3$ .

The proposed  $\text{NO}_x$  capture and utilization system was integrated into the exhaust stream of an  $\text{NH}_3$ -fired combined-cycle power plant, as shown in Figure 1. In the integrated system, a premixed gaseous flow of  $\text{NH}_3$  fuel, dry air, and recirculated exhaust gas (EGR) is first compressed and introduced into a primary combustor, which undergoes high-temperature combustion. This process generates thermal energy for electricity production via a gas turbine. However, the elevated combustion temperature also facilitates the formation of thermal and fuel  $\text{NO}_x$ . If unreacted  $\text{NH}_3$  remains after the primary combustion stage—particularly under fuel-rich conditions—the remaining  $\text{NH}_3$  is directed into a secondary combustor, where additional air is introduced to ensure complete combustion. In this secondary stage, combustion occurs at a comparatively lower temperature. Notably, the remaining  $\text{NH}_3$  can also chemically reduce a portion of the previously generated  $\text{NO}_x$ , resulting in partial  $\text{NO}_x$  neutralization. Following secondary combustion, the high-temperature exhaust gas is utilized to transfer heat to a water-based coolant loop, which produces steam to drive a steam turbine and generate additional electricity. Finally, the cooled exhaust gas with the remaining  $\text{NO}_x$  enters the  $\text{NO}_x$  absorber unit, where  $\text{NO}_x$  is captured and converted into  $\text{KNO}_3$ , thereby detoxifying the exhaust gas. A portion of the treated gas is recirculated as EGR to improve system efficiency and temperature control. Thus, this integrated system co-produces electricity and chemical material,  $\text{KNO}_3$ .

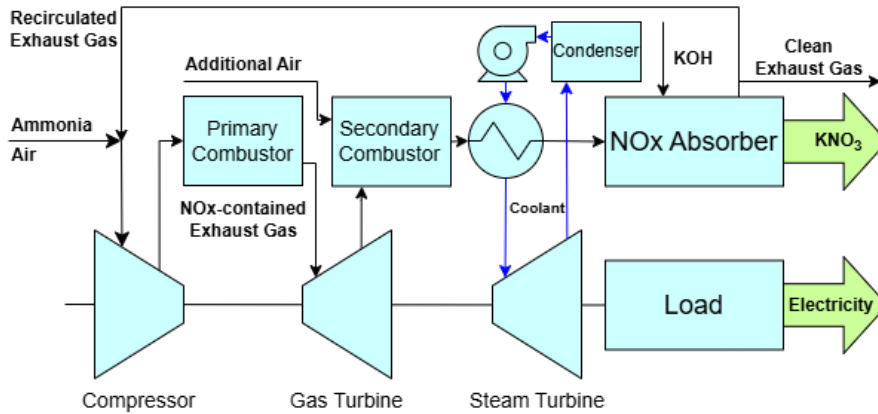


Figure 1: The schematic illustration of the proposed co-production system.

### 3. Method

In this research, a simulation study followed by an economic comparison between different  $\text{NH}_3$ -to-air conditions was conducted to demonstrate the difference in value produced from  $\text{NO}_x$  utilization for evaluation of the proposed system.

A lab-scale experiment for  $\text{KNO}_3$  synthesis from nitrogen gas containing 500 ppm  $\text{NO}_2$  was conducted in a previous study (Ino et al., 2025) to demonstrate the feasibility of the proposed  $\text{NO}_x$  absorber shown in Figure 1. The experimental results provided the necessary data for simulating the performance of the proposed system. The findings indicated that the  $\text{NO}_x$  absorption ratio ( $\eta_A$ )—defined as the proportion of  $\text{NO}_x$  removed by the absorbent relative to the  $\text{NO}_2$  content in the incoming gas—exceeded 75%. However,  $\eta_A$  decreased to 43% as the absorbent became neutralized. Meanwhile, the product conversion ratio ( $\eta_p$ )—defined as the mass of  $\text{KNO}_3$  formed relative to the theoretical value based on the stoichiometric consumption of  $\text{KOH}$ —was found to be 96%. In the subsequent calculations,  $\eta_A = 75\%$  and  $\eta_p = 96\%$  were adopted as performance parameters. These experimental values were adopted to evaluate the effectiveness of the proposed system in this research.

#### 3.1 Simulation setup

An  $\text{NH}_3$ -fired thermal power plant was simulated using AVEVA PRO/II Simulation 2024 software. The system configuration shown in Figure 1 was implemented in the simulation flowchart presented in Figure 2. This configuration was used to assess both the power plant's performance and the amount of  $\text{NO}$  produced.

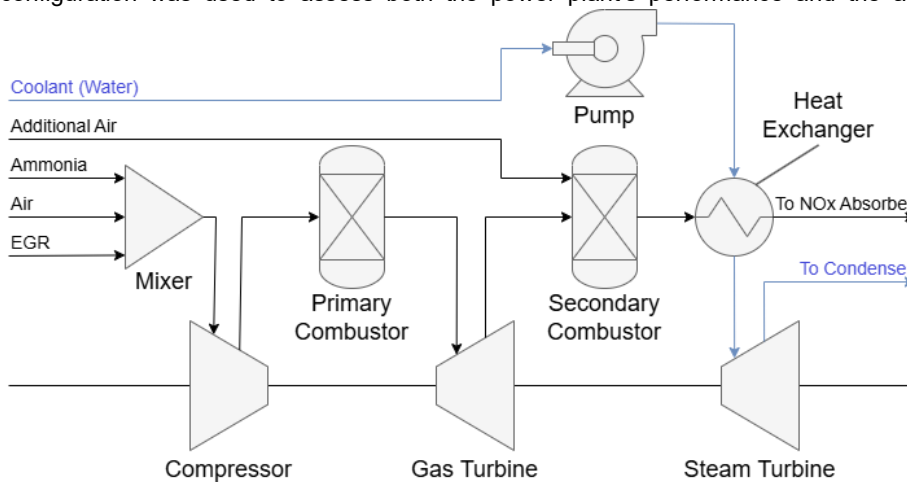


Figure 2: The simulation flowchart of the proposed co-production system.

All gaseous inputs were supplied at a temperature of 25 °C and a pressure of 101.325 kPa. The flow rate of  $\text{NH}_3$  ( $F_{\text{AMMONIA}}$ ) as shown Ammonia in Figure 2 was fixed at 100 kmol/h of  $\text{NH}_3$ , while the inflow air to the compressor with  $\text{NH}_3$  was assumed to be standard dry air, consisting of 78.08% nitrogen, 20.95% oxygen, 0.93% of argon, and 0.04% of  $\text{CO}_2$ . The air flow rate ( $F_{\text{AIR}}$ , in kmol/h) to the combustor was calculated based on the equivalence

ratio (ER:  $\epsilon$ ), defined as the ratio of the actual fuel(NH<sub>3</sub>)-to-air ratio to the stoichiometric fuel(NH<sub>3</sub>)-to-air ratio. Accordingly,  $F_{AIR}$  was derived using Eq(1).

$$F_{AIR} = \frac{3}{4} \times \frac{100}{\epsilon \times 20.95 \%} = \frac{75}{\epsilon \times 20.95 \%} \quad (1)$$

where 3/4 is the stoichiometric ratio for complete combustion of NH<sub>3</sub>, shown as Eq(2) below.



The EGR inflow increases the inlet gas temperature while suppressing the peak combustion temperature, thereby preventing excessive thermal stress in the combustor without altering the ER. In the simulation, as the component and thermal property of exhaust gas rely on the NH<sub>3</sub> combustion and NO<sub>x</sub> absorption conditions, the flow of EGR was simulated with pure nitrogen gas at 25 °C and 101.325 kPa corresponding to the conditions in NO<sub>x</sub> absorber, and its flow rate was adjusted to maintain the combustor temperature at the target value.

When ER exceeds 1, the combustion of NH<sub>3</sub> becomes incomplete, leading to unburned NH<sub>3</sub> that may cause NH<sub>3</sub> slip when released into the atmosphere. To prevent such cases, an inflow of standard dry air with sufficient flowrate was introduced to the secondary combustor to ensure complete combustion of the remaining NH<sub>3</sub>.

The circulation of coolant was also simulated with pure water inflow. The water was supplied at 25 °C and 5 kPa, and its flowrate was set so the steam turbine's vapor temperature reached the target temperature.

Table 1 summarizes the assumptions made for the remaining system components. The temperatures and pressures for the combustor and steam turbine were based on the gas turbines and the supercritical steam turbines that have already been put into practical use. All flows between components and combustion reactors were assumed to be adiabatic. As NO forms from the combustion of NH<sub>3</sub> as Eq(3) and NO<sub>2</sub> is produced from the oxidation of NO through the system, the NO<sub>x</sub> formation ratio from NH<sub>3</sub> combustion was referred to the NO conversion ratio ( $\eta_{NO}$ ) in the primary combustor under different ER values provided by JST-LCS (2018).



Table 1: Power generation conditions for the simulation model.

Name	Value	Name	Value
Combustor temperature	1,627 °C	Compressor adiabatic efficiency	85 %
Steam temperature	600 °C	Turbine adiabatic efficiencies	85 %
Compressor compression ratio	25	Pump efficiency	80 %
Steam pumped pressure	25 MPa	Heat exchanger	50 °C
Steam final pressure	5 kPa	minimum temperature difference	

### 3.2 Economic evaluation

The simulation results were used to evaluate and compare the economic value generated per unit of NH<sub>3</sub> consumed, taking into account both electricity generation and material production. The amount of electricity generated was calculated as the network output, defined as the difference between the work (all in kW) produced by the gas turbine ( $W_G$ ) and steam turbine ( $W_S$ ) and the work consumed by the pump ( $W_P$ ) and compressor ( $W_C$ ). It was assumed that no energy losses occurred in power generation. The amount of material (KNO<sub>3</sub>) produced was estimated based on the referred NO<sub>x</sub> conversion ratio  $\eta_{NO}$  and the previously determined absorption and conversion ratios,  $\eta_A$  and  $\eta_P$ .

Both the electricity and material outputs were then converted into monetary values to enable comparison across different ERs. The revenue from electricity generation ( $V_E$ , in JPY/kmol-NH<sub>3</sub>) was calculated using an electricity price ( $p_E$ ) of 30.0 JPY/kWh, corresponding to the home electricity (low voltage) price level in Japan (TEPCO 2023). The net value of the material produced ( $V_P$ , in JPY/kmol-NH<sub>3</sub>) was calculated using the commercial prices of KOH ( $p_{KOH}$ ) at 14.6 JPY/mol (METI, 2023) and KNO<sub>3</sub> ( $p_{KNO_3}$ ) at 55.1 JPY/mol (Plants Corp., 2023). The calculation methods are presented in Eqs(4) and (5).

$$V_E = \frac{(W_G + W_S - W_P - W_C) p_E}{F_{AMMONIA}} \quad (4)$$

$$V_P = \eta_{NO} \eta_A \eta_P (p_{KNO_3} - p_{KOH}) \times 10^3 \quad (5)$$

## 4. Results and Discussions

### 4.1 Simulation outcomes

Figure 3 and Table 2 present the simulation results at different ERs. The electricity generated per unit of  $\text{NH}_3$  combusted was slightly higher at ERs below 1. In contrast,  $\text{NO}_x$  emissions at ERs greater than one were significantly reduced due to the unburned  $\text{NH}_3$  reacting with  $\text{NO}_x$  within the combustor. For this reason, previous studies have preferred combustion conditions around ER 1.1–1.2 to minimize post-treatment costs associated with  $\text{NO}_x$  emissions.

When ER is lower, the presence of excess oxygen in the combustor increases  $\text{NO}_x$  formation. The additional  $\text{NO}_x$  enables greater  $\text{KNO}_3$  production in the proposed system, thereby generating higher economic returns per unit of  $\text{NH}_3$  combusted at lower ERs.

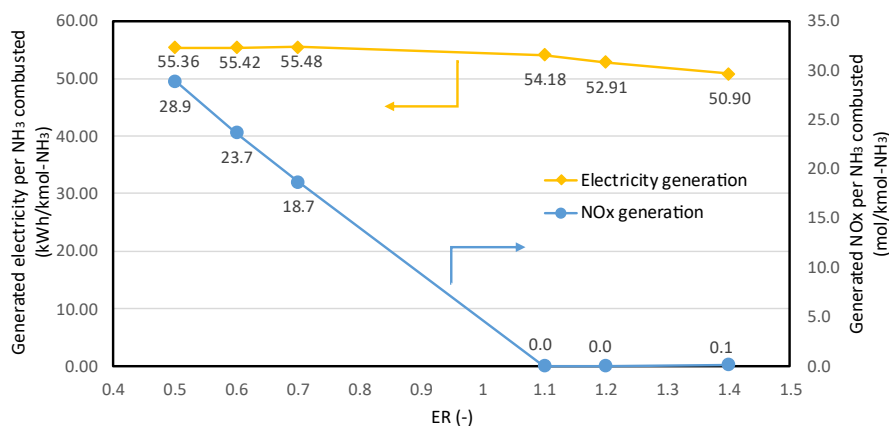


Figure 3: Simulated results of electricity and  $\text{NO}_x$  produced at different ERs.

Table 2: Simulation results of flowrates and works at different ERs.

ER(-)	$\eta_{\text{NO}}$ (%)	$F_{\text{EGR}}$ (kmol/h)	$F_{\text{COOLANT}}$ (kmol/h)	$W_P$ (kW)	$W_C$ (kW)	$W_G$ (kW)	$W_S$ (kW)
0.5	2.89	104.2	446.8	70.1	3,850.0	6,501.9	2,954.5
0.6	2.37	226.3	447.4	70.2	3,862.8	6,517.1	2,958.2
0.7	1.87	313.9	448.0	70.3	3,873.6	6,530.1	2,961.8
1.1	0.00	411.8	467.4	73.3	3,499.6	5,899.9	3,090.6
1.2	0.00	360.0	481.8	75.6	3,163.3	5,343.8	3,185.7
1.4	0.01	278.7	504.5	79.1	2,635.5	4,469.6	3,335.4

### 4.2 Economic evaluation

Based on the simulation results,  $V_E$  and  $V_P$  were calculated for each ER using Eqs(4) and (5) to allow for direct comparison. Figure 4 illustrates the net economic value per unit of  $\text{NH}_3$  combusted, derived from electricity generation and  $\text{KNO}_3$  production.

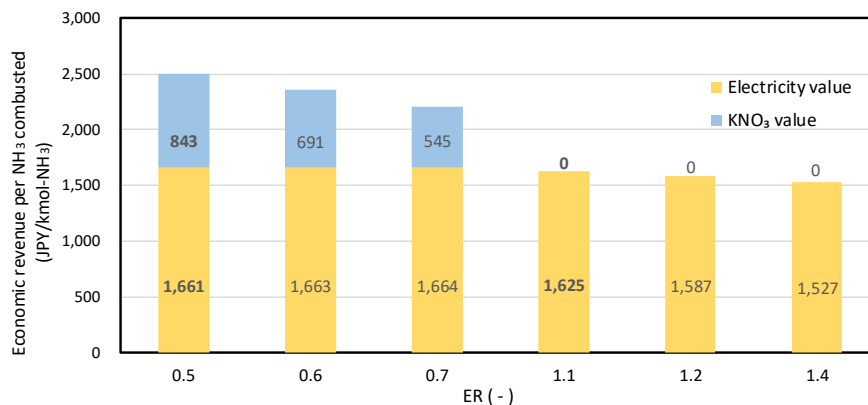


Figure 4: Economic values from electricity and  $\text{KNO}_3$  produced at different ERs.

Compared to low-NO<sub>x</sub> combustion at ER 1.1, the utilization of NO<sub>x</sub> in the exhaust gas led to a substantial increase in overall economic value when the proposed system was applied. At ER 0.5, the profit from KNO<sub>3</sub> production alone accounted for approximately 52 % of the electricity profit at ER 1.1. In addition, electricity output slightly improved (by 1 %) due to a higher contribution from the gas turbine than from the steam turbine. Overall, a 53 % increase in total economic return was observed for ER 0.5 compared to ER 1.1, underscoring the strong potential of the proposed system as an effective chemical recycling and value-enhancing solution.

## 5. Conclusions

Utilizing NO<sub>x</sub>-containing exhaust gas to synthesize valuable materials offers a promising approach to offset NO<sub>x</sub> treatment costs and generate additional profit through chemical recycling. However, the economic potential of the recovered material depends on both the concentration of NO<sub>x</sub> and the purity of other acidic gases in the exhaust. Therefore, this study conducted a preliminary investigation into the feasibility and economic effectiveness of a proposed KOH-based NO<sub>x</sub> capture and utilization system, integrated into an NH<sub>3</sub>-fired combined-cycle power plant.

A simulation-based analysis was conducted to evaluate both power generation and NO<sub>x</sub> production under various operating conditions. The resulting electricity and material outputs were then translated into economic values to assess profitability across different ERs. The results demonstrated that, for the same amount of NH<sub>3</sub> combusted, operation at ER 0.5 led to increased electricity output and significant KNO<sub>3</sub> production. Under the assumed system and economic conditions, this translated to a 53 % increase in total profit compared to low-NO<sub>x</sub> combustion at ER 1.1, primarily driven by the value of the coproduced KNO<sub>3</sub>.

In summary, these preliminary findings suggest that the proposed NO<sub>x</sub> capture and utilization system is a highly feasible chemical recycling approach and holds considerable promise for further development and commercial deployment.

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