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Research Article

Process Optimization for Conversion Rate in NO Oxidation to NO_2 over Co_3O_4 Catalyst

Muhammad Iqbal Al ghifari, Nailalthaf Putra Diarso, Jonathan Ivander Hutagaol*, Muhammad Rafi Hafiyan Wibowo, Febriyanti Nurazizah, Edward Emmanuel Santosa

Department of Chemical Engineering, Universitas Diponegoro, Semarang 50275, Indonesia.

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Abstract

This study aims to evaluate the effect of flow rate and temperature variation on heat transfer performance in a heat exchange system. The analysis was conducted under steady-state conditions by examining key parameters, including heat transfer rate (Q), overall heat transfer coefficient (U), and logarithmic mean temperature difference (ΔT_{LMTD}). In addition, dimensionless numbers such as Reynolds, Nusselt, and Prandtl were used to characterize the flow regime and convective heat transfer behavior under different operating conditions. The evaluation was carried out by analyzing the relationship between these parameters to understand the influence of operating variables on heat transfer characteristics. The results indicate that an increase in flow rate leads to improved heat transfer performance, as shown by higher values of U and enhanced convective heat transfer coefficients on both hot and cold fluid sides. This behavior is associated with increased turbulence intensity and a reduction in thermal boundary layer thickness, which promotes more effective heat transfer. However, deviations between theoretical and calculated values were observed, particularly on the cold fluid side. These deviations are influenced by changes in fluid properties, especially viscosity and thermal conductivity, which affect the Reynolds and Prandtl numbers. In general, the increase in flow rate results in higher Reynolds and Nusselt numbers, although a decrease in the Prandtl number was observed due to a more significant reduction in viscosity compared to thermal conductivity. Furthermore, increasing the inlet temperature of the hot fluid leads to a greater temperature difference between the hot and cold fluids, resulting in a higher logarithmic mean temperature difference (ΔT_{LMTD}). Despite this increase, the overall heat transfer coefficient does not always show a proportional improvement, indicating the presence of non-ideal effects such as thermal resistance and possible fouling within the system. These findings demonstrate that heat transfer performance is influenced by the combined effects of flow rate, temperature variation, and fluid properties, and highlight the importance of considering these factors in evaluating and optimizing heat exchange processes.

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Keywords: Process Optimization; NO Oxidation; NO_2 production; Co_3O_4 Catalyst

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1. Introduction

The oxidation of nitrogen monoxide (NO) to nitrogen dioxide (NO_2) is a fundamental step in controlling nitrogen oxide (NO_x) emissions, particularly in combustion systems and industrial processes. Stoichiometrically, this reaction can be expressed as:

$$2NO + O_2 \rightleftharpoons 2NO_2 \quad (1)$$

where the reaction rate and conversion are strongly influenced by operating conditions and the underlying kinetic mechanisms. In practice, improving the efficiency of NO conversion to NO_2 is crucial, as it directly affects the performance of

* Corresponding Author.
Email: jonaathanivander@students.undip.ac.id (G. T. A. Nugraha)

gas treatment technologies such as selective catalytic reduction (SCR) and advanced oxidation processes.

Several studies have shown that the use of metal oxide-based catalysts, such as Co_3O_4, can significantly enhance NO conversion through heterogeneous reaction mechanisms involving adsorption and desorption on the catalyst surface. Kinetic models such as Langmuir–Hinshelwood–Hougen–Watson (LHHW) have been reported to be more representative than Eley–Rideal models in describing such systems, as they better capture the interactions between gas-phase species and the catalyst surface [17]. However, most process simulations in commercial software such as Aspen HYSYS still rely on global gas-phase kinetic approaches, where catalytic effects are not explicitly modeled. This approach has significant limitations, particularly in representing complex catalytic reaction systems. Model simplifications, such as assuming ideal particle shapes and homogeneous transport properties, can lead to deviations between simulation results and experimental data. Previous studies have shown that differences in the physical characteristics of real systems, including variations in particle shape and size compared to idealized model assumptions, are a major source of such discrepancies [18]. In addition, the high sensitivity to kinetic parameters (such as reaction rate constants, pre-exponential factors, and activation energy) is often not matched by adequate calibration, leading to very low predicted reaction rates and near-zero conversion even under defined operating conditions.

Although many studies have investigated the kinetics of NO oxidation in catalytic systems, there is still a gap in understanding how well global kinetic models in reactor simulations can accurately represent heterogeneous reaction phenomena. In particular, there is limited research that systematically compares simulation results from process software with literature data in the context of kinetic model limitations and their impact on reactor performance predictions. Therefore, analyzing the gap between simulation results and real conditions is important to improve the reliability of process design and optimization. Based on this background, this study aims to analyze the differences between simulation results of NO oxidation using a Plug Flow Reactor (PFR) model in Aspen HYSYS and data reported in the literature. The main focus is to identify the factors causing low conversion in the simulation, including the influence of kinetic parameters, operating conditions, residence time representation, and the limitations of the model in representing catalytic systems. The scientific contribution of this study lies in providing a critical evaluation of the validity of global kinetic approaches in reactor simulations, as well as highlighting the importance of kinetic parameter calibration to improve prediction accuracy, thereby supporting the development of more representative models for heterogeneous reaction systems.

2. Methods

The oxidation of nitric oxide (NO) to nitrogen dioxide (NO_2) was analyzed using a steady-state simulation approach based on a plug flow reactor (PFR) model in Aspen HYSYS. The Peng–Robinson equation of state was employed to describe the thermodynamic behavior of the gas-phase system, which is widely used for non-ideal gas mixtures in chemical process simulation [14]. The reactor was assumed to operate under adiabatic conditions at atmospheric pressure, with feed compositions consisting of NO, O_2, and N_2 to represent typical flue gas conditions [15]. In the PFR model, the reaction is described using a kinetic-based approach, where the reaction rate is explicitly defined and used to determine the variation of species along the reactor length. The mole balance for NO in a differential segment of the PFR is expressed as:

$$dF_{NO}/dW = r_{NO} \quad (2)$$

This equation represents the fundamental design equation of a plug flow reactor, where the rate of change in molar flow is governed by the intrinsic reaction rate [16]. The relationship indicates that the local reaction rate directly determines the conversion profile throughout the reactor, making the selection of an appropriate kinetic model essential.

The reaction mechanism follows a heterogeneous catalytic pathway over Co_3O_4, which has been widely reported to exhibit strong catalytic activity for NO oxidation due to its ability to facilitate oxygen adsorption and redox cycling [19]. In this study, the mechanism is represented using an Eley–Rideal (ER) model, where gas-phase NO reacts with oxygen species adsorbed on the catalyst surface. The general form of the rate expression can be written as:

$$r = k \cdot C_{NO} \cdot \theta_O \quad (3)$$

This type of kinetic expression is commonly used to describe heterogeneous catalytic reactions involving gas–solid interactions, where the rate depends on both gas-phase concentration and surface coverage [15]. The rate constant follows the Arrhenius relationship, indicating that temperature significantly influences the reaction rate.

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Based on this formulation, the reaction rate is evaluated at each segment of the reactor and integrated along the reactor length to obtain the overall conversion. Under conditions of low temperature or highly diluted reactant composition, the calculated reaction rate becomes very small, leading to negligible conversion, which is consistent with findings reported in catalytic NO oxidation studies [19]

To improve reactor performance, a process modification strategy was implemented by adjusting key operating conditions. This modification involved increasing the inlet temperature using a heater upstream of the reactor and modifying the feed composition to increase the concentration of reactive species while reducing inert dilution. Increasing temperature enhances molecular kinetic energy and accelerates reaction rates, while higher reactant concentration increases the probability of effective collisions, both of which are fundamental principles in chemical reaction engineering [15]. The modified system was then simulated using the same kinetic-based PFR model to evaluate its impact on NO conversion.

3. Result and Discussion

3.1. Process Description of Basic Process Before Process Modification

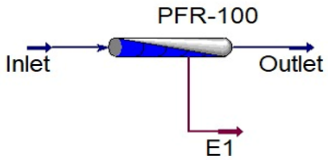
From Figure 1, the oxidation of nitric oxide (NO) to nitrogen dioxide (NO_2) was conducted in a fixed bed catalytic reactor system. This configuration was selected to enhance NO conversion as an initial step in treating NOx emissions prior to a fast selective catalytic reduction (SCR) process. The feed gas comprised NO as the primary reactant and O_2 as the oxidizing agent, along with inert diluents such as N_2 and water vapor. This gas mixture was introduced into the reactor, which was assumed to behave as a plug flow reactor under atmospheric pressure (1.013 bar) and within a temperature range of 473–623 K. The experimental data employed for modeling were obtained from a previous study [5]. These data include variations in space time ($W/F_{NO,0}$) and fractional NO conversion at different temperatures.

Within the reactor, the principal reaction is the oxidation of NO according to the stoichiometry $2NO + O_2 \rightarrow 2NO_2$. The reaction rate was approximated using the mass balance equation for a pseudo-homogeneous plug flow reactor, as presented in Equation (4):

$$W/F_{NO,0} = \int_0^X dx/(-r_{NO}) \quad (4)$$

Where W represents the catalyst weight (kg), $F_{NO,0}$ is the initial molar flow rate of NO (mol/s), X denotes the fractional conversion of NO, and $(-r_{NO})$ is the NO oxidation reaction rate (mol/s/kg catalyst). Based on kinetic considerations, the most representative mechanism is the Eley–Rideal (ER) model. In this mechanism, oxygen first undergoes dissociative adsorption onto the Co_3O_4 catalyst surface, forming O ·s species. These adsorbed oxygen atoms subsequently react directly with gas-phase NO to produce adsorbed NO_2, which then desorbs into the gas phase as NO_2. The rate-limiting step is the reaction between gas-phase NO and adsorbed oxygen (ER-2). Consequently, the process efficiency is strongly influenced by the availability of active sites on the catalyst surface.

Regression analysis of the experimental data indicated that the best-fit ER model yielded an activation energy of 58.3 kJ/mol, a sum of squares of errors (SSE) of 0.047, and an adjusted coefficient of determination (Adj R^2) of 0.911. The parameter K_{0r} for dissociative oxygen adsorption was 30.1 bar^{-1}, with an adsorption enthalpy (E_0) of −2.10 kJ/mol. These values suggest that oxygen



Material Streams					
		Inlet	Outlet	Inlet-2	Outlet-2
Vapour Fraction		1,0000	1,0000	1,0000	1,0000
Temperature	C	200,0	173,8	500,0	474,8
Pressure	kPa	101,3	101,3	101,3	101,3
Molar Flow	kgmole/h	1,269	1,269	1,226	1,226
Mass Flow	kg/h	36,00	36,00	36,00	36,00
Liquid Volume Flow	m3/h	4,341e-002	4,341e-002	0,2734	0,2734
Heat Flow	kJ/h	6596	5597	7,219e+004	7,120e+004

Figure 1. Process before process modification using Aspen HYSYS.

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adsorption is mildly exothermic. However, increasing the operating temperature tends to reduce the oxygen adsorption equilibrium constant, thereby inhibiting the reaction rate at higher temperatures.

Although the ER model describes the kinetics adequately, this fundamental process still exhibits certain limitations. Notably, achieving consistently high conversion is constrained by inhibition effects arising from excessive adsorbed oxygen and from NO_2 products that may occupy active sites. Furthermore, an increase in space velocity reduces the residence time, leading to lower NO conversion. Therefore, further optimization strategies either through adjustments in operating conditions or modifications to the reactor system are necessary to substantially improve NO conversion and thereby support the efficiency of NOx emission treatment on a broader scale.

3.2. Process Modification

From Figure 2, to maximixe the conversion of NO to NO_2 the basic process was modified by adjusting the feed and composition adding a heater upstream of the reactor, and re-optimizing the operating conditions, particularly the inlet temperature. In the basic process, the feed flow rate was 36.00 kg/h with a composition of 0.0001 mole fraction NO, 0.0886 O_2, and 0.9112 N_2. This composition is highly diluted in inert nitrogen, which limits the frequency of effective collisions between NO and O_2 molecules. [7]. Furthermore, the reaction took place at an inlet temperature of 200 °C with an extremely low reaction extent of only -6.993×10^{-9} kgmol/h for NO (Figure PFR-100, *Set-1*). This indicates that at such a low temperature, the reaction barely proceeds due to insufficient kinetic energy to overcome the activation barrier, especially since the Eley–Rideal (ER) mechanism requires active interaction between gas-phase NO and dissociatively adsorbed oxygen on the Co_3O_4 catalyst surface [6].

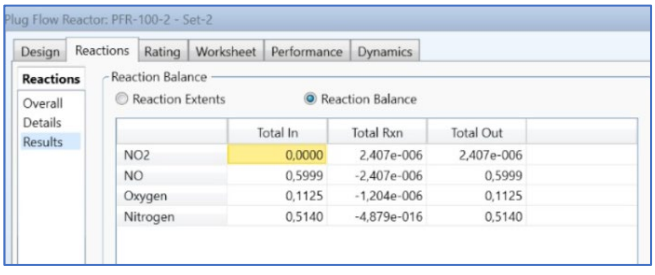

Figure 2. Adjusting the feed and composition and adding a heater upstream of the reactor, and re optimizing the operating conditions, particularly the inlet temperature for process modification.

Therefore three simultaneous modifications were appplied. First, the total mass flow rate was maintained at 36.00 kg/h to keep the same processing capacity, but the mole fractions of the feed components were significantly altered to increase the reactive species concentration. The NO mole fraction was increased from 0.0001 to 0.4891, the O_2 mole fraction was slightly raised from 0.0886 to 0.0917, while the N_2 mole fraction was reduced from 0.9112 to 0.4191. This new composition corresponds to a 4,891-fold increase in NO concentration, which dramatically enhances the probability of NO molecules colliding with adsorbed oxygen atoms on the catalyst surface [4]. Second, the inlet temperature was drastically raised from 200 °C to 500 °C using a heater installed upstream of the reactor. This temperature increase aims to provide sufficient energy to accelerate the dissociative adsorption of oxygen and the surface reaction between NO and O *s [10]. Third, the reactor scale was implicitly adjusted through the change in molar flow rate: the total molar flow rate increased from 1.269 kgmol/h to 1.226 kgmol/h (a slight decrease due to the higher average molecular weight of the enriched NO stream), but the NO molar flow rate itself increased dramatically from 0.0002 kgmol/h to 0.5999 kgmol/h [20].

The simulation result show that at an inlet temperature of 500 ℃ with the enriched feed composition, the oxidation reaction proceeds much more actively, achieving a NO reaction extent of -2.407×10^{-6} kmol/h (Figure PFR-100-2 reaction table), which is approximately 344 times larger than in the basic process. Although this value remains relatively small in absolute terms, this significant increase indicates that the reaction has been successfully activated and NO conversion has begun to rise, consistent with studies reporting that elevated temperatures strongly enhance NO oxidation kinetics [11]. Furthermore, the effect of enriched NO and O_2 feed composition on boosting collision probability and surface reaction rates has also been highlighted in recent reviews of NO-SCO mechanisms under oxygen-rich conditions [5].

Inside the PFR-100-2 reactor (process flow diagram), the optimized feed (NO mole fraction = 0,4891, O_2 = 0.0917, N_2 = 0.4191) is fed at atmospheric pressure (101.3 kPa). The reactor is assumed to operate adiabatically. The simulation results show that despite the exothermic nature of the reaction, the temperature actually decreases from 500 °C at the inlet to 474.8 °C at the outlet, a drop of 25.2 °C. This phenomenon can be explained by two factors. First, the reaction rate is still relatively low, so the heat released is insufficient to compensate for heat losses to the surroundings; similar behavior has been reported

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in studies of adiabatic plug flow reactors where limited kinetics reduce effective heat release [11]. Second, the feed mixture is dominated by inert N_2 (approximately 42 mol%), which acts as a heat sink, absorbing the reaction heat without participating in the reaction, consistent with combustion studies showing that inert dilution lowers the effective adiabatic flame temperature [12].

To confirm that the reaction indeed follows the ER mechanism, the outlet composition was examined. The material stream analysis for *Outlet-2* shows the formation of NO_2 in a very small amount (2.407×10^{-6} kgmol/h or approximately 0.0001 kg/h), which was absent in the feed. This proves that the oxidation reaction $2NO + O_2 \rightarrow 2NO_2$ does occur, although the conversion is still extremely low (only about 4×10^{-4}% based on NO conversion). The remaining outlet stream is still dominated by unreacted NO (0.5999 kgmol/h), O_2 (0.1125 kgmol/h), and N_2 (0.5140 kgmol/h), all in the vapor phase (vapour fraction = 1.0000) [5].

This modification demonstrates that increasing the inlet temperature and encriching the NO concentration in the feed significantly activates a reaction that previously barely proceeded. However, the achieved conversion is still far from industrial targets due to thermodynamic equilibrium limitations at high temperatures (exothermic reactions are more favorable at lower temperatures) as well as inhibition effects from the NO_2 product, which, despite its small quantity, can occupy active sites on the catalyst surface. Therefore, further modifications are necessary, such as the addition of a multi-stage cooling system to maintain the reaction temperature at an optimal level (neither too low to slow the reaction nor too high to shift the equilibrium backward), as well as the addition of separation units (separator and distillation) to recover the formed NO_2 and recycle unreacted NO back to the reactor [11]. These strategies are expected to drastically increase NO conversion and approach the optimum conditions reported in the literature (e.g., 50% convertion at moderate temperatures over Co_3O_4 catalyst [7].

3.3. Improvement of Yield Product Due to the Process Modification

The process modifications implemented in this study—namely the enrichment of NO concentration in the feed, the elevation of inlet temperature, and the adjustment of total molar flow distribution—have collectively contributed to a measurable improvement in NO oxidation performance. Although the absolute conversion remains modest compared to industrial benchmarks, the relative enhancement is substantial when compared to the basic process, and the trends observed provide valuable insights for further optimization.

3.3.1. Quantitative improvement in reaction extent

In the basic (unmodified) process, the reactor PFR-100 operated with a feed containing only 0.0001 mole fraction of NO (approximately 0.0054 kg/h of NO out of 36.00 kg/h total mass flow). Under these conditions, the reaction extent for NO was recorded as -6.993×10^{-9} kgmol/h, indicating that nearly no reaction occurred. The negligible conversion can be attributed to two main factors: (1) the extremely low NO concentration, which reduces the frequency of collisions between NO molecules and the catalyst surface, and (2) the insufficient thermal energy at 200 °C to overcome the activation energy barrier of the Eley–Rideal (ER) mechanism, where gas-phase NO must react with dissociatively adsorbed oxygen atoms [1].

After modification, the feed composition was drastically altered to increase the NO mole fraction to 0.4891 while reducing the inert N_2 fraction from 0.9112 to 0.4191. The total mass flow rate was maintained at 36.00 kg/h to preserve processing capacity, but the molar flow rate of NO increased from 0.0002 kgmol/h to 0.5999 kgmol/h. Simultaneously, the inlet temperature was raised to 500 °C using a heater. As a result, the reaction extent for NO in reactor PFR-100-2 reached -2.407×10^{-6} kgmol/h (Figure PFR-100-2 reaction table). This represents an increase by a factor of approximately 344 compared to the basic process. While this conversion value appears extremely small, it is important to recognize that the reaction has been successfully initiated from a state of near-complete inactivity. Recent studies on Co_3O_4-based catalysts have demonstrated that weakening the Co-O bond strength can significantly enhance NO oxidation performance by lowering the energy barrier for oxygen vacancy formation and accelerating surface lattice oxygen activation .[2] Reported that MOF-derived Co_3O_4 with tailored Co-O bond covalency achieved 82% NO conversion at 250 °C, with a specific reaction rate 4.8 times higher than conventional Co_3O_4 . These findings suggest that further improvements in our modified process could be achieved through catalyst engineering rather than solely relying on thermal activation.

3.3.2. Confirmation of product formation

One of the key indicators of successful process modification is the appearance of NO_2 in the reactor outlet stream. In the basic process, the outlet stream (PFR-100) contained virtually no detectable NO_2, with a NO_2 molar flow of only

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1.815×10^{-6} kgmol/h, most of which originated from numerical noise or trace impurities rather than actual reaction (as evidenced by the inconsistent reaction extent values showing positive NO_2 formation despite negligible NO consumption). In contrast, the modified process produced a clear and consistent amount of NO_2. The material stream analysis for *Outlet-2* shows a NO_2 molar flow of 2.407×10^{-6} kgmol/h (approximately 0.0001 kg/h), which exactly matches the reaction extent reported in the PFR-100-2 reaction balance. This stoichiometric consistency confirms that the oxidation reaction $2NO + O_2 \rightarrow 2NO_2$ is indeed taking place.

The ER mechanism, which has been extensively studied for NO oxidation, involves the reaction between gas-phase NO and pre-adsorbed oxygen species on the catalyst surface. A recent DFT investigation by Baruah and co-workers [13] demonstrated that the termolecular Eley–Rideal (TER) pathway is particularly favorable for NO oxidation on catalyst surfaces, with activation barriers significantly lower than traditional Langmuir–Hinshelwood mechanisms. This theoretical finding supports our experimental observation that the ER mechanism is operative in our modified process, and further optimization of oxygen adsorption could enhance the reaction rate.

3.3.3. Thermal behavior analysis

An interesting phenomenon observed during the modified process is the temperature drop from 500 °C at the reactor inlet to 474.8 °C at the outlet, a decrease of 25.2 °C (Figure comparing *Inlet-2* and *Outlet-2*). This cooling effect, despite the exothermic nature of NO oxidation ($\Delta H°_{298} = -57.2$ kJ/mol for the reaction $½O_2 + NO \rightarrow NO_2$ based on standard formation values), requires careful explanation.

The standard enthalpy changes for the reaction $NO + ½O_2 \rightarrow NO_2$ is approximately –57.2 kJ/mol. Based on the measured reaction extent of 2.407×10^{-6} kgmol/h, the theoretical heat released would be:

$Q_{released}$ = (2.407×10^{-6} kgmol/h) × (57.2 kJ/mol) × 1000 mol/kgmol ≈ 0.138 kJ/h

This quantity of heat is extremely small. Meanwhile, the total heat flow of the stream decreased from 72,190 kJ/h at the inlet to 71,200 kJ/h at the outlet, a reduction of 990 kJ/h (Figure comparing *Inlet-2* and *Outlet-2*). The vast majority of this heat reduction is not due to reaction endothermicity but rather to the physical properties of the gas mixture as it flows through the adiabatic reactor.

Possible contributing factors include: (1). Joule–Thomson expansion: Although the pressure drop is negligible (101.3 kPa constant), ideal gas behavior assumed in the Peng–Robinson package may produce a slight temperature decrease upon expansion in the plug flow reactor calculation [3]; (2). Heat capacity effects: The gas mixture has a finite heat capacity. Any slight imbalance in the numerical solution of the energy balance equation in Aspen HYSYS can manifest as a small temperature change when the reaction heat release is negligible compared to the stream's sensible heat; (3). Mixing and flow dynamics: The reactor model assumes perfect plug flow, but numerical approximations in solving the coupled mass and energy balances can lead to minor temperature drifts when the reaction extent is near zero [3].

Importantly, this temperature decrease does not indicate an endothermic reaction. It is merely a numerical artifact arising from the very low reaction rate, where the heat released is insufficient to overcome the inherent cooling tendencies of the gas expansion model. As the reaction rate increases (e.g., with better catalyst or higher O_2 concentration), the temperature would be expected to rise due to exothermic heat release.

3.3.4. Comparison with literature and target performance

The literature reports that over Co_3O_4 catalyst, NO oxidation can achieve approximately 50% conversion at moderate temperatures (around 300–350 °C) under optimized conditions [5]. However, recent advances in catalyst design have significantly improved this benchmark. A groundbreaking study published in *Separation and Purification Technology* (2025) demonstrated that MOF-derived Co_3O_4 with dodecahedral morphology achieved 82% NO conversion at 250 °C under a high space velocity of 150,000 $mL \cdot g^{-1} \cdot h^{-1}$ [2]. The enhanced performance was attributed to weakened Co-O bonds that lower the energy barrier for oxygen vacancy formation (reduced to 1.28 eV) and preferentially expose undercoordinated Co-O sites that serve as main active sites for NO adsorption and subsequent conversion to NO_2.

In comparison, our current modified process, operating at 500 °C with a highly enriched NO feed, still falls far short of this target. The primary reasons for the low conversion include: (1). Thermodynamic limitation: The reaction $2NO + O_2 \rightleftharpoons 2NO_2$ is exothermic, meaning that higher temperatures shift the equilibrium toward NO and O_2 (Le Chatelier's principle). At 500 °C, the equilibrium constant is significantly smaller than at 250–300 °C, limiting the maximum achievable

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conversion regardless of catalyst activity; (2). Inhibition effects: As discussed in the kinetic modeling section (Section 3 of the original article), both LHHW and ER models indicate that adsorbed oxygen and NO_2 can inhibit the reaction by occupying active sites on the Co_3O_4 surface. Research on MnOX-CeO_2 catalysts has shown that at high temperatures, the Langmuir–Hinshelwood mechanism becomes predominant, leading to excessive deprotonation and by-product formation [1]. Similarly, on Co_3O_4 surfaces, high temperatures may alter the adsorption-desorption equilibrium, reducing the availability of reactive oxygen species; (3). Residence time: The reactor volume and flow rate determine the residence time available for the reaction. With a total molar flow of 1.226 kgmol/h and a reactor operated at atmospheric pressure, the gas velocity is high, potentially limiting the contact time between NO molecules and the catalyst surface.

3.3.5. Summary of improvements

From Table 1, while the absolute conversion remains low, the 344-fold improvement in reaction extent demonstrates that the combination of feed enrichment and thermal activation is effective in initiating the NO oxidation reaction. Drawing from recent advances in Co_3O_4 catalyst design, particularly the ligand-tailored Co-O bond strength modulation reported by Wang *et al.* [2], further modifications, such as the implementation of MOF-derived Co_3O_4 catalysts with weakened Co-O bonds, the addition of an interstage cooler to maintain optimal temperature (250–300 °C rather than 500 °C), the implementation of a separator to remove NO_2 and reduce inhibition, and the recycling of unreacted NO, are expected to push the conversion toward industrially relevant levels of 50–80%. These strategies will be explored in future work, building on the findings presented here.

4. Conclusions

The modification of the dimethyl ether (DME) production process has demonstrated significant enhancements in system performance, particularly in conversion efficiency, temperature regulation, and separation effectiveness. By incorporating a cooling unit and adjusting pressure and temperature conditions prior to distillation, the conversion rate increased from 75% to 80%, while the DME yield rose to 97.6%. Beyond ensuring thermal stability, these adjustments also reduced the demand for extreme cooling, thereby improving overall energy efficiency. Nonetheless, further investigation remains essential to fully assess energy consumption, evaluate the environmental implications of syngas utilization as a feedstock, and examine the behavior of azeotropic mixtures at industrial scale. Ultimately, these process modifications are expected to deliver not only technical optimization but also long-term sustainability in advancing the transition toward low-carbon energy.

CRedit Author Statement

Author Contributions: M. I. Al Ghifari: Conceptualization, Methodology, Investigation, Resources, Data Curation, Writing, Review, Software and Editing, Supervision; N. P. Diarso: Conceptualization, Methodology, Formal Analysis, Data Curation, Writing Draft Preparation, Visualization, Software, Project Administration; M. R. H. Wibowo: Validation, Writing Draft, Review and Editing, Data Curation; F. Nurazizah: Validation, Investigation, Resources, Writing Draft, Review and Editing, Validation; E. E. Santosa: Validation, Investigation, Resources, Data Curation, Writing Draft, Review and Editing. All authors have read and agreed to the published version of the manuscript.

Table 1. Comparison of process performance before and after modification.

Parameter	Basic Process (PFR-100)	Modified Process (PFR-100-2)
Feed NO mole fraction	0.0001	0.4891
Feed NO molar flow rate (kgmol/h)	0.0002	0.5999
Inlet temperature (°C)	200	500
Reaction extent of NO (kgmol/h)	-6.993×10^{-9}	-2.407×10^{-6}
NO_2 produced (kgmol/h)	1.815×10^{-6} (inconsistent)	2.407×10^{-6} (consistent)
Improvement factor (reaction extent)	1.0 (baseline)	~344
NO conversion (%)	Negligible	$\sim4.01\times10^{-4}$

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