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Recent advances in modelling and experimental studies of SCR catalysts in ammonia-fuelled engine applications

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Ammonia (NH_3) has emerged as a promising carbon-free fuel for decarbonising internal combustion engines and power systems. However, its combustion produces elevated nitrogen oxide (NO_x) emissions and ammonia slip, requiring effective exhaust aftertreatment. Selective catalytic reduction (SCR) is the leading technology for NO_x control, but its application to ammonia-fuelled engines presents unique challenges, including NH_3-rich exhaust, variable NO_2:NO_x ratios, low exhaust gas temperatures (EGT), high water-vapour concentrations, and increased potential for nitrous oxide (N_2O) formation. This review critically examines recent advances in SCR catalyst development and modelling for ammonia-combustion exhaust treatment. The performance of vanadia-based catalysts, transition metal oxides, and Cu- and Fe-exchanged zeolites (CuZ and FeZ) is evaluated in terms of activity, selectivity, durability, and resistance to deactivation under ammonia-rich conditions. Current understanding of NH_3-SCR reaction mechanisms, catalyst ageing, and N_2O formation is discussed alongside advances in microkinetic, reactor-scale, and computational fluid dynamics (CFD) modelling. Particular emphasis is placed on the strong coupling between combustion and aftertreatment, arising from the dual role of NH_3 as both fuel and reductant, and the need to integrate experimental observations with predictive modelling. Finally, key research priorities are identified, including catalyst development for NH_3-rich exhaust, realistic experimental validation, improved prediction of N_2O emissions, and integrated combustion–aftertreatment optimisation to enable efficient, low-emission NH_3-fuelled power and propulsion systems.

KEYWORDS
ammonia-fuelled, experimental, modelling, NOx emissions, selective catalytic reduction (SCR), zeolite

1 Introduction

The urgent need to reduce greenhouse gas emissions and transition toward sustainable energy systems has intensified interest in alternative carbon-free fuels. Among these, ammonia (NH_3) has emerged as a promising candidate due to its high hydrogen (H_2) density, established production and distribution infrastructure, and potential for carbon-neutral synthesis (Mørch et al., 2011; Okafor et al., 2019). Unlike conventional hydrocarbon fuels, NH_3 combustion does not produce carbon dioxide (CO_2); however, it introduces significant challenges associated with pollutant formation, particularly nitrogen oxides (NO_x) and unburned NH_3.

NH_3 combustion in internal combustion engines is characterised by low laminar burning velocities (LBV), narrow flammability limits, and high ignition energy

requirements, often resulting in incomplete combustion and elevated NH_3 slip (Liu et al., 2023; Mørch et al., 2011). Experimental studies on NH_3-fuelled and NH_3 dual-fuel (DF) engines have demonstrated that NO_x emissions remain a major challenge despite the absence of carbon-containing exhaust species (Lesmana et al., 2021; Reiter and Kong, 2011). These characteristics distinguish NH_3-fuelled systems from conventional diesel and gasoline engines and necessitate dedicated aftertreatment strategies.

Selective catalytic reduction (SCR) technology remains the most effective technology for NO_x abatement under lean-burn conditions. Conventionally, SCR systems rely on NH_3 generated from aqueous urea (NH_2CONH_2) decomposition. In NH_3-fuelled engines, however, residual NH_3 present in the exhaust may partially or completely replace external reductant dosing under certain operating conditions (Lesmana et al., 2019; Cardoso et al., 2021). This creates opportunities for simplified aftertreatment architectures but also introduces challenges associated with controlling NH_3 slip, catalyst selectivity, and N_2O formation.

The composition of NH_3-combustion exhaust differs substantially from that of conventional diesel engines. Variations in $NO:NO_2$ ratios, high water vapour concentrations, fluctuating NH_3 slip levels, and comparatively low exhaust gas temperatures (EGT) can significantly alter catalyst performance and reaction pathways (Abu-Jrai et al., 2017; Kuta et al., 2023). Consequently, catalyst formulations originally developed for diesel applications may not operate optimally under NH_3-fuelled conditions.

Several candidate aftertreatment architectures have been proposed for NH_3-fuelled engines, differing in catalyst arrangement and the utilisation of engine-out NH_3 slip. Figure 1 summarises representative configurations currently being explored. Depending on the combustion strategy and engine-out exhaust composition, systems may incorporate combinations of diesel oxidation catalysts (DOC), SCR catalysts, ammonia slip catalysts (ASC), and dedicated N_2O decomposition catalysts. Unlike conventional urea-SCR systems, NH_3-fuelled engines may utilise engine-out NH_3 slip as the reductant, reducing or eliminating the need for external urea dosing. The most suitable architecture depends on engine operating conditions, catalyst performance, and emissions-control requirements.

Significant advances have been made in SCR catalyst development over the past 2 decades. Vanadia-based catalysts remain widely used due to their high activity within the 300 °C–450 °C temperature range (Busca et al., 1998). More recently, Cu- and Fe-exchanged zeolites (CuZ and FeZ) have gained prominence because of their superior hydrothermal stability and broader operating windows (Guo Y, 2017; Paolucci et al., 2017). Detailed

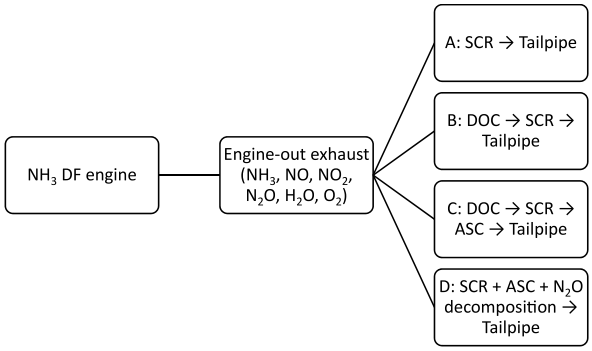


FIGURE 1
Representative candidate exhaust aftertreatment architectures for NH_3-fuelled engines.

spectroscopic and kinetic studies have revealed the critical role of redox-active metal centres, Brønsted acidity, and NH_3 storage capacity (NSC) in governing catalyst activity and selectivity.

Advances in experimental characterisation techniques, including operando spectroscopy, transient reactor studies, and isotopic labelling experiments, have substantially improved understanding of SCR reaction pathways. These studies have identified key surface intermediates involved in NH_3 activation and NO_x reduction, supporting mechanistic descriptions based on Langmuir–Hinshelwood (L-H), Eley-Rideal (E-R), and Mars-van Krevelen (MvK) pathways (Paolucci et al., 2017; Ramis et al., 1996).

In parallel, modelling approaches have evolved from empirical kinetic expressions to detailed microkinetic and reactor-scale simulations. Modern SCR models incorporate NH_3 adsorption, surface reactions, diffusion limitations, and transient storage phenomena, enabling prediction of catalyst performance under realistic engine operating conditions (Olsson et al., 2008; Song et al., 2015). Computational fluid dynamics (CFD) models have further enhanced understanding of flow distribution, reductant mixing, and temperature non-uniformities within full-scale aftertreatment systems. Despite these advances, relatively few studies have coupled combustion and aftertreatment models specifically for NH_3-fuelled engines, where exhaust composition differs markedly from conventional applications.

An additional challenge arises from the formation of nitrous oxide (N_2O), a potent greenhouse gas (GHG) with a global warming potential (GWP) approximately 273 times greater than that of CO_2 over a 100-year timescale (IPCC, 2021). Experimental investigations have shown that N_2O formation depends strongly on catalyst composition, operating temperature, and the $NO_2:NO_x$ ratio at the SCR inlet (Jung et al., 2022; Madia et al., 2002). Under NH_3-rich conditions typical of NH_3 combustion, side reactions involving NH_3 oxidation and NH_4NO_3 decomposition can significantly increase N_2O emissions.

While reviews such as Gopinathan and Mohamed Ibrahim, 2025 have examined NH_3 combustion strategies and engine performance, comparatively less attention has been given to the behaviour of SCR catalysts under sustained NH_3-rich exhaust conditions and the associated mechanisms of N_2O formation. This review provides a comprehensive assessment of recent advances in experimental and

Abbreviations: ASC, Ammonia slip catalyst; CFD, Computational fluid dynamics; CHA, Chabazite; DOC, Diesel oxidation catalyst; DFT, Density functional theory; DPF, Diesel particulate filter; DRIFTS, Diffuse reflectance infrared fourier transform spectroscopy; E-R, Eley-Rideal; EATS, Exhaust aftertreatment system; EGT, Exhaust gas temperature; GHSV, Gas hourly space velocity; L-H, Langmuir–Hinshelwood; LBV, Laminar burning velocity; MvK, Mars-van Krevelen; NH_3-SCR, Ammonia selective catalytic reduction; NSC, NH_3 storage capacity; SCR, Selective catalytic reduction; TPD, Temperature-programmed desorption; XAS, X-ray absorption spectroscopy.

TABLE 1 SCR reaction pathways.

SCR pathway	Overall balanced reaction	Typical conditions	Potential issues
Standard SCR	$4NH_3 + 4NO + O_2 \rightarrow 4N_2 + 6H_2O$	NO-dominant exhaust (NO_2:NO_x < 0.5)	Most common pathway in diesel and NH_3 engines. Slower at low temperature
Fast SCR	$2NH_3 + NO + NO_2 \rightarrow 2N_2 + 3H_2O$	NO:NO_2 ≈ 1:1	Most efficient SCR pathway, particularly below 300 °C. NO_2 availability
NO_2-SCR (slow SCR)	$4NH_3 + 3NO_2 \rightarrow 3.5N_2 + 6H_2O$	NO_2-rich exhaust	Promotes NH_4NO_3 formation at low temperatures
NH_3 oxidation (desired)	$4NH_3 + 3O_2 \rightarrow 2N_2 + 6H_2O$	High temperature; ASC or oxidative SCR catalysts	Removes excess NH_3 while producing N_2
NH_3 oxidation (undesired NO formation)	$4NH_3 + 5O_2 \rightarrow 4NO + 6H_2O$	High temperature; highly oxidative catalysts	Reduces NH_3 availability and forms additional NO.
NH_3 oxidation (undesired N_2O formation)	$2NH_3 + 2O_2 \rightarrow N_2O + 3H_2O$	NH_3-rich, oxidative conditions	Major secondary greenhouse-gas formation pathway

modelling studies of SCR catalysts for NH_3 combustion exhaust treatment. Particular emphasis is placed on catalyst materials, reaction mechanisms, kinetic modelling approaches, and the coupling between combustion processes and catalytic aftertreatment. By critically examining current developments and identifying remaining research gaps, this review aims to support the development of robust, efficient, and low-emission SCR systems for future NH_3-based engine applications.

2 Characteristics of ammonia combustion exhaust

NH_3 combustion produces an exhaust composition that differs fundamentally from that of conventional hydrocarbon-fuelled engines, creating unique challenges and opportunities for SCR systems. While the absence of carbon eliminates direct CO_2 emissions, combustion of NH_3 introduces substantial concentrations of nitrogen-containing species, including NO_x and unburned NH_3, which strongly influence catalyst performance and aftertreatment design. In addition, exhaust temperature, oxygen (O_2) concentration, water vapour content, and the presence of reactive intermediates can significantly alter SCR reaction pathways and catalyst selectivity (Kobayashi et al., 2019; Valera-Medina et al., 2018). Engine-out temperature and exhaust composition are key design parameters for NH_3-based SCR systems because they directly influence catalyst activity and sizing, and NH_3 utilisation (Kuta et al., 2022).

2.1 NO_x formation and speciation

Unlike hydrocarbon combustion, where NO_x is predominantly formed through thermal-NO mechanisms, NO_x formation during NH_3 combustion is largely governed by fuel-bound nitrogen chemistry. NH_3 oxidation proceeds through a complex network of elementary reactions involving NH_2, NH, N, HNO and N_2H_x intermediates, which ultimately lead to the formation of NO and NO_2 (Glarborg, 2022; Kobayashi et al., 2019). Consequently, NH_3-fuelled engines often exhibit higher engine-out NO_x emissions than conventional diesel engines, particularly under stoichiometric and moderately lean conditions where fuel-nitrogen conversion is favoured (Valera-Medina et al., 2018).

The relative proportions of NO and NO_2 are critical for SCR performance. In conventional diesel exhaust, NO typically dominates, whereas NH_3 combustion can lead to more variable NO:NO_2 ratios depending on combustion conditions and post-combustion oxidation processes (Kobayashi et al., 2019). The presence of NO_2 is beneficial for the "fast SCR" reaction, where an equimolar NO:NO_2 ratio enhances reaction rates, extends catalyst activity to lower temperatures, and improves overall NO_x conversion efficiency (Brandenberger et al., 2008). The NO:NO_2 ratio produced during NH_3 combustion is particularly important for downstream SCR performance. Conditions that generate a balanced NO:NO_2 ratio enhances fast-SCR activity and improves low-temperature NO_x conversion, whereas NO-dominated exhaust generally relies on the slower standard-SCR pathway (Koebel et al., 2000; Song et al., 2015). However, excessive NO_2 concentrations may promote undesirable side reactions, including the formation of ammonium nitrate (NH_4NO_3) and subsequent N_2O emissions, particularly under low-temperature operating conditions (Madia et al., 2002). Reactor-scale studies have demonstrated that SCR performance is highly sensitive to inlet NO_2:NO_x ratios and temperature-dependent transitions between standard SCR, fast SCR and NH_3 oxidation pathways, highlighting the importance of accurately representing coupled transport and reaction kinetics in predictive models (Wang et al., 2020). SCR reaction pathways are summarised in Table 1.

2.2 Ammonia slip and its dual role

A defining characteristic of NH_3-fuelled engines is the presence of significant unburned NH_3 in the exhaust stream. NH_3 possesses a low LBV, high autoignition temperature, and relatively slow

oxidation kinetics, all of which contribute to incomplete combustion and NH_3 slip, especially under low-load and lean-burn operation (Lesmana et al., 2021; Valera-Medina et al., 2018).

From an emissions perspective, NH_3 slip is undesirable due to the toxicity of NH_3 and its contribution to secondary particulate formation in the atmosphere. However, from an aftertreatment perspective, the presence of NH_3 represents a potentially valuable intrinsic reductant for SCR. Unlike conventional diesel SCR systems that rely on urea decomposition to generate NH_3, NH_3-fuelled engines may provide sufficient NH_3 directly from combustion, reducing or potentially eliminating the need for external reductant dosing (Kuta et al., 2023).

This concept, often referred to as passive SCR, has attracted considerable attention because it simplifies aftertreatment architecture and reduces system complexity. Nevertheless, experimental investigations have demonstrated that the engine-out NH_3 concentration is highly dependent on operating conditions and is frequently insufficient to achieve complete NO_x conversion across the entire engine map (Lesmana et al., 2021). Consequently, strategies such as fuel bypass, supplementary NH_3 injection, or adaptive catalyst control may still be required. The exhaust NH_3:NO_x ratio is of particular importance for downstream SCR operation. Experimental studies have reported optimum SCR performance at NH_3:NO_x ratios of approximately 1–1.4, indicating that combustion conditions producing balanced NO_x and NH_3 slip may reduce the external urea demand of the aftertreatment system (Zhao et al., 2023).

Excessive NH_3 slip presents an additional challenge because downstream ammonia slip catalysts (ASC) may oxidise NH_3 to NO, NO_2, or N_2O instead of the desired N_2, thereby creating secondary emissions (Ramis et al., 1996; Schaber et al., 2004). ASC should not be viewed solely as NH_3 cleanup devices; under NH_3-rich exhaust conditions they can influence NOx conversion and N_2O formation simultaneously, making them an integral component of future NH_3-engine aftertreatment architectures (Wu et al., 2024). Balancing NO_x reduction efficiency against NH_3 slip therefore represents a key optimisation challenge for NH_3-fuelled SCR systems.

2.3 Exhaust gas temperature characteristics

Exhaust gas temperature (EGT) is one of the most influential parameters governing SCR performance. Compared with conventional diesel combustion, NH_3 combustion often produces lower adiabatic flame temperatures, particularly under lean-burn conditions and in NH_3-H_2 or NH_3-diesel DF operation (Valera-Medina et al., 2018).

As a result, exhaust temperatures frequently fall within the low-temperature region where SCR activity is kinetically limited. Temperatures below approximately 200 °C–250 °C reduce NH_3 activation and slow both adsorption and surface reaction rates, leading to poor NO_x conversion efficiency (Brandenberger et al., 2008; Damma et al., 2019). This challenge is particularly relevant during cold-start operation, low-load engine conditions, and auxiliary power applications.

Conversely, high-temperature operation introduces a different limitation. Above approximately 450 °C–500 °C, NH_3 oxidation reactions become increasingly competitive with SCR reactions, resulting in decreased NO_x conversion efficiency and increased formation of NO and N_2O (Nicosia et al., 2008). Maintaining catalyst operation within an optimal temperature window is therefore essential for achieving high N_2 selectivity.

The combination of low-temperature activity requirements and high-temperature stability demands has driven significant interest in Cu- and Fe-exchanged zeolites (CuZ and FeZ), which exhibit broader operational windows than conventional vanadia-based catalysts (Damma et al., 2019).

2.4 Presence of additional reactive species

NH_3 combustion exhaust contains several additional species that can influence SCR chemistry. Residual oxygen is typically present because NH_3 engines often operate under lean conditions to suppress NO_x formation and improve combustion stability (Valera-Medina et al., 2018).

O_2 plays a dual role in SCR systems. Moderate O_2 concentrations promote oxidation of NO to NO_2, thereby facilitating fast-SCR pathways and improving low-temperature activity. However, excessive O_2 availability can also accelerate NH_3 oxidation, reducing NH_3 utilisation efficiency and increasing N_2O formation (Kuta et al., 2023).

H_2 may also be present, particularly in NH_3-H_2 DF engines or in systems where NH_3 cracking is employed to enhance combustion. Residual H_2 can modify catalyst surface chemistry and, under suitable conditions, promote H_2-assisted SCR pathways that improve low-temperature NO_x conversion (Liu et al., 2011).

Water vapour represents another important exhaust constituent. Although generally considered a weak inhibitor, water can compete with NH_3 and NO_x species for adsorption sites, particularly at lower temperatures, thereby reducing catalyst activity (Madia et al., 2002). Long-term exposure to high water concentrations may also accelerate hydrothermal ageing of zeolite catalysts, resulting in framework degradation and loss of active metal sites (Paolucci et al., 2017).

In NH_3 DF engines, trace hydrocarbons originating from pilot fuels may also be present. These species can compete for active sites and alter catalyst selectivity, particularly under low-temperature conditions where hydrocarbon adsorption is favoured (Olsson et al., 2008).

2.5 Implications for SCR system design

The unique characteristics of NH_3 combustion exhaust necessitate a fundamentally different approach to SCR system design compared with conventional diesel applications. The simultaneous presence of NO_x and NH_3 creates opportunities for passive SCR operation, but also introduces challenges associated with NH_3 slip control, N_2O formation, and catalyst selectivity.

Catalysts must therefore exhibit:

- High activity at low exhaust temperatures;
- Strong resistance to hydrothermal ageing;
- High N_2 selectivity under NH_3-rich conditions;
- Low NH_3 oxidation activity;

TABLE 2 Key characteristics of NH_3 combustion exhaust and their implications for SCR performance.

Characteristic	Effect on SCR system
High NO_x concentrations from fuel-nitrogen chemistry	Increases demand for catalyst activity and reductant availability
Variable NO:NO_2 ratio	Strongly influences standard and fast-SCR reaction rates
NH_3 slip	Provides intrinsic reductant but risks NH_3 emissions and N_2O formation
Lower exhaust temperatures	Reduces low-temperature catalyst activity and NO_x conversion
Residual O_2	Promotes fast-SCR but can accelerate NH_3 oxidation
Water vapour	Competes for adsorption sites and contributes to catalyst ageing
Residual H_2	May enhance low-temperature NO_x reduction through H_2-assisted pathways
Transient engine operation	Requires robust catalyst control and adaptive modelling approaches

- Minimal N_2O formation across a wide operating window.

These requirements increasingly favour advanced zeolite catalysts and hybrid catalyst architectures capable of maintaining performance under highly variable exhaust conditions (Damma et al., 2019; Paolucci et al., 2017). Furthermore, because engine-out NH_3 and NO_x concentrations are strongly influenced by combustion strategy, SCR optimisation cannot be considered independently of engine calibration. Integrated combustion-aftertreatment approaches are therefore emerging as a key research direction for NH_3-fuelled powertrains. The key characteristics of ammonia combustion exhaust and their implications for SCR performance are summarised in Table 2.

3 SCR catalyst technologies for ammonia combustion exhaust

SCR catalysts are central to achieving efficient NO_x abatement in NH_3-fuelled systems. However, the distinct characteristics of NH_3 combustion exhaust, particularly NH_3 fuel-rich conditions, variable NO:NO_2 ratios, and lower exhaust gas temperatures (EGT), place additional demands on catalyst performance. Consequently, catalyst selection must consider not only activity and selectivity, but also physicochemical properties such as redox behaviour, NH_3 storage capacity (NSC), and resistance to deactivation.

3.1 Catalyst families

A comparison of major SCR catalyst families for ammonia combustion exhaust is provided in Table 3.

3.1.1 Vanadia-based catalysts

Vanadia-based catalysts, typically formulated as V_2O_5-WO_3/TiO_2, remain among the most widely deployed commercial SCR catalysts owing to their high NO_x conversion efficiency and N_2 selectivity within an intermediate temperature window of approximately 300 °C–450 °C (Busca et al., 1998; Nova et al., 2009). Their activity arises from the coexistence of Brønsted and Lewis acid sites that facilitate NH_3 adsorption and activation, together with redox-active vanadium species that promote NO_x reduction via surface O_2 transfer reactions.

TABLE 3 Comparison of major SCR catalyst families for ammonia combustion exhaust (Brandenberger et al., 2008; Damma et al., 2019; Gao et al., 2013).

Catalyst family	Typical formulation	Active temperature window (°C)	Key advantages	Main limitations	Suitability for NH_3-fuelled engines
Vanadia-based	V_2O_5–WO_3/TiO_2	300–450	High NO_x conversion, excellent N_2 selectivity, industrial maturity	Limited low-temperature activity, vanadium toxicity, NH_3 oxidation at high temp	Moderate
Cu-zeolite (CuZ)	Cu-SSZ-13, Cu-SAPO-34	180–450	Excellent low-temperature activity, high NH_3 storage capacity	N_2O formation under NH_3-rich conditions, hydrothermal aging	High
Fe-zeolite (FeZ)	Fe-ZSM-5, Fe-BEA	300–600	High-temperature stability, good durability	Lower low-temperature activity	High
MnO_x-based	MnO_x/TiO_2	100–250	Excellent low-temperature activity	Poor N_2 selectivity, SO_2 sensitivity	Moderate
CeO_2-based	CeO_2-containing mixed oxides	150–400	High O_2 storage capacity, water tolerance	Stability and selectivity challenges	Moderate
PGM-based	Pt, Pd, Rh	150–500	High oxidation activity	High cost, N_2O formation	Mainly ASC applications

However, their applicability to NH_3 combustion exhaust is limited by poor low-temperature activity and increased NH_3 oxidation at elevated temperatures. Under NH_3-rich conditions, these side reactions can decrease N_2 selectivity and promote formation of NO and N_2O (Jung et al., 2022). Long-term operation at high temperatures may also lead to vanadium volatilisation and catalyst deactivation through sintering and phase transformations of both the active phase and support (Guan et al., 2014; Nova et al., 2009).

3.1.2 Zeolite-based catalysts

Metal-exchanged zeolites have become the dominant SCR technology for modern automotive and stationary applications owing to their wide operating temperature windows and superior hydrothermal stability (Fickel and Lobo, 2010; Gao et al., 2013). Among these materials, Cu-CHA and Fe-ZSM-5 catalysts have received particular attention because of their excellent activity under fuel-lean conditions. SCR activity in CuZ and FeZ is associated with isolated exchanged metal ions and well-dispersed active centres, rather than metal oxide clusters.

Cu-exchanged zeolites exhibit outstanding low-temperature SCR activity and high NH_3 storage capacity (NSC) due to the presence of isolated Cu^{2+} ions and mobile Cu species that participate in rapid Cu^{2+}/Cu^{+} redox cycling (Paolucci et al., 2017). Consequently, CuZ are particularly attractive for NH_3-fuelled engines, where lower exhaust temperatures are often encountered. FeZ generally exhibit lower low-temperature activity but maintain high NO_x conversion at temperatures above 450 °C and display superior thermal stability under severe operating conditions (Brandenberger et al., 2008; Gao et al., 2013; Shin et al., 2020 reported NOx conversion above approximately 80% between about 300 °C and 450 °C for both catalyst systems in non-road engines.

Recent spectroscopic and computational studies have demonstrated that catalyst performance depends strongly on the coordination environment and mobility of exchanged metal ions within the zeolite framework, which directly influence SCR reaction pathways and catalyst durability (Borfecchia et al., 2015; Paolucci et al., 2017).

3.1.3 Transition metal oxide catalysts

Vanadium-free transition metal oxides have attracted increasing attention as environmentally benign alternatives to conventional SCR catalysts. Among these materials, manganese oxides exhibit exceptional low-temperature activity due to the coexistence of multiple oxidation states (Mn^{2+}, Mn^{3+} and Mn^{4+}), which facilitate rapid redox cycling and oxygen transfer reactions (Chen et al., 2012; Zhang et al., 2023). Several studies have reported NO_x conversions exceeding 90% below 250 °C. However, their strong oxidation capability often promotes NH_3 overoxidation, resulting in poor N_2 selectivity and increased N_2O formation.

Ceria-based catalysts have emerged as promising candidates because of their high O_2 storage capacity and reversible Ce^{4+}/Ce^{3+} redox cycle. These properties enhance O_2 mobility, improve resistance to water inhibition, and promote catalytic stability under transient operating conditions (Zhou et al., 2021). Iron oxide catalysts generally exhibit moderate activity over a broader temperature range but remain limited by lower low-temperature performance compared with Mn- and Cu-based systems.

3.1.4 Platinum group metal (PGM) catalysts

Platinum group metals (Pt, Pd and Rh) exhibit exceptionally high intrinsic catalytic activity and are widely employed in NH_3 oxidation catalysts and ammonia slip catalysts (ASCs). Their ability to activate NH_3 at low temperatures makes them highly effective for downstream NH_3 removal.

Nevertheless, the strong oxidation activity of PGMs often leads to poor N_2 selectivity at elevated temperatures, with significant formation of NO and N_2O (Lott and Deutschmann, 2023). Combined with their high cost and susceptibility to poisoning, these limitations have restricted their use as primary SCR catalysts. Instead, PGMs are increasingly incorporated into hybrid catalyst architectures that combine efficient NO_x reduction with downstream NH_3 oxidation functionality.

3.2 Key physicochemical characteristics

The performance of SCR catalysts is governed not only by their chemical composition but also by a range of physicochemical properties that influence adsorption, reaction kinetics, mass transport, and long-term stability. These characteristics are particularly important in NH_3-fuelled applications, where exhaust composition and operating conditions differ substantially from conventional diesel systems.

SCR activity is strongly influenced by the synergy between redox-active centres responsible for NO oxidation and acidic sites responsible for NH_3 adsorption and activation, highlighting the importance of balancing redox and acidity characteristics during catalyst design (Liu et al., 2014). High SCR activity requires an appropriate balance between acidity and redox capability rather than maximizing either property independently (Shi et al., 2023). One of the most important parameters is the nature and distribution of active sites. SCR reactions require the adsorption and activation of NH_3 on Brønsted and Lewis acid sites, followed by reaction with adsorbed NO_x species. The relative abundance and strength of these sites influence NH_3 storage, reaction rates, and selectivity. For example, Cu-exchanged CHA zeolites contain isolated Cu ions capable of participating in rapid redox cycles while simultaneously providing strong NH_3 adsorption capacity, contributing to their excellent low-temperature activity (Paolucci et al., 2017). High dispersion of active metal species has been identified as a critical factor governing NH_3-SCR activity, as dispersed sites provide greater accessibility and promote efficient redox cycling compared with bulk oxide phases. The performance of NH_3-SCR catalysts is governed not only by intrinsic redox activity but also by the synergistic interaction between redox centres and Brønsted/Lewis acid sites, with highly dispersed active species providing the most effective balance of NH_3 adsorption, NO oxidation, and catalytic turnover. Brønsted and Lewis acid sites are not merely NH_3 storage sites but actively participate in different NH_3 activation pathways, leading to different SCR reaction routes and kinetics (Nova et al., 2009). The distribution and strength of

TABLE 4 Key physicochemical properties governing SCR performance.

Property	Role in SCR	Influence on performance
Brønsted acidity	NH_3 adsorption as NH_4^+	Enhances NH_3 storage and SCR activity
Lewis acidity	NH_3 coordination and activation	Promotes NH_2 intermediate formation
Redox activity	NO oxidation and catalyst turnover	Improves SCR rates, especially fast SCR
O_2 mobility	Lattice O transport	Influences NH_3 oxidation and N_2O formation
NH_3 storage capacity (NSC)	NH_3 buffering during transients	Improves conversion but may increase NH_3 slip
Pore structure	Diffusion of reactants/intermediates	Controls mass-transfer limitations
Hydrothermal stability	Resistance to thermal aging	Determines catalyst lifetime
Sulphur tolerance	Resistance to sulphation	Critical for long-term operation

Brønsted and Lewis acid sites strongly influence NH_3 adsorption, storage, activation and overall SCR activity, making acidity a key design parameter for next-generation catalysts (Shi et al., 2023).

Redox properties are equally important because NO oxidation and catalyst regeneration depend on the ability of active species to undergo reversible oxidation–reduction cycles. Catalysts with high oxygen mobility and readily accessible lattice oxygen generally exhibit enhanced SCR activity, particularly under transient conditions. Ceria-based materials are notable in this regard due to the reversible Ce^{4+}/Ce^{3+} redox couple, which promotes oxygen storage and oxygen mobility and NO oxidation capability, promoting the fast SCR pathway and extending catalytic activity over a broader temperature range, while improving resistance to fluctuations in exhaust composition (Zhang et al., 2023).

NH_3 storage capacity (NSC) strongly influences catalyst performance during transient operation. High NH_3 storage enables the catalyst to buffer short-term variations in NH_3 availability and maintain NO_x conversion during rapid changes in engine load. However, excessive NH_3 storage may increase the risk of NH_3 slip if stored NH_3 is subsequently released under changing operating conditions (Song et al., 2015).

The pore structure and morphology of the catalyst also play a critical role. Zeolitic catalysts possess highly ordered microporous structures that provide large surface areas and abundant adsorption sites, but diffusion limitations may arise at high gas hourly space velocities (GHSV). In contrast, mesoporous materials generally offer improved mass transport but lower adsorption capacity. Consequently, an appropriate balance between adsorption strength and diffusion accessibility is required to maximise catalyst utilisation under realistic exhaust conditions (Busca et al., 1998).

Long-term catalyst durability depends largely on resistance to hydrothermal ageing, sulphur poisoning, and thermal degradation. Exposure to high temperatures and water vapour can induce framework collapse, metal agglomeration, or phase transformations that reduce active-site availability. Sulphur-containing species may additionally block active sites through sulphate formation, particularly in catalysts exposed to pilot-fuel combustion products. Among current SCR catalyst families, Cu-CHA materials generally exhibit superior hydrothermal stability, whereas vanadia-based catalysts are more susceptible to thermal degradation at elevated temperatures (Brandenberger et al., 2008; Damma et al., 2019).

Collectively, these physicochemical properties determine the activity, selectivity, and durability of SCR catalysts and therefore represent critical design parameters for NH_3-fuelled engine applications. The key physiochemical properties governing SCR performance are summarised in Table 4.

3.3 Catalyst requirements for ammonia combustion exhaust

The exhaust composition produced by NH_3-fuelled engines imposes a set of catalyst requirements that differ significantly from those encountered in conventional diesel applications. In addition to achieving high NO_x conversion, catalysts must tolerate elevated concentrations of unburned NH_3, large variations in EGT, high water vapour levels, and changing NO: NO_2 ratios while maintaining high selectivity towards N_2.

A primary requirement is strong low-temperature activity. NH_3 combustion generally produces lower EGT than diesel combustion, particularly under lean and low-load operation (Valera-Medina et al., 2018). Consequently, SCR catalysts must remain active below 250 °C, where conventional vanadia-based systems often exhibit limited performance. This requirement has driven substantial interest in Cu-exchanged zeolites, which can achieve high NO_x conversion efficiencies under low-temperature conditions through enhanced NH_3 storage and fast-SCR activity (Paolucci et al., 2017; Damma et al., 2019).

Catalysts must also effectively accommodate substantial fluctuations in NH_3 concentration. Unlike conventional SCR systems that rely on controlled urea dosing, NH_3-fuelled engines inherently produce varying levels of NH_3 slip depending on combustion strategy, load, and fuel substitution ratio. This creates opportunities to utilise residual NH_3 as the SCR reductant, reducing or potentially eliminating external urea injection. However, successful implementation requires catalysts capable of maintaining high conversion efficiency over a broad range of NH_3:NO_x ratios while minimising secondary NH_3 emissions (Kuta et al., 2023; Lesmana et al., 2021).

Selectivity towards N_2 is another critical consideration. Under NH_3-rich conditions, competing reactions such as NH_3 oxidation and NH_4NO_3 decomposition may increase emissions of N_2O and

NO, reducing the environmental benefits of NH_3 as a carbon-free fuel. Consequently, catalyst formulations must be designed to maximise N_2 formation while suppressing undesired by-products. This challenge is particularly important during low-temperature operation, where N_2O formation pathways become increasingly significant (Jung et al., 2022).

The high-water content of NH_3 combustion exhaust additionally requires catalysts with strong hydrothermal stability and resistance to water inhibition. Water vapour can compete with reactants for adsorption sites and accelerate catalyst ageing through framework degradation or metal migration. Similarly, the use of pilot fuels may introduce sulphur-containing species that promote sulphate formation and catalyst deactivation. Recent research has therefore focused on hydrothermally stable zeolite frameworks, hydrophobic surface modifications, and sulphur-tolerant transition metal oxides capable of maintaining activity under prolonged exposure to realistic exhaust environments (Brandenberger et al., 2008; Zhang et al., 2023). Recent studies show that hydrothermal aging affects Brønsted and Lewis acid sites differently, leading to progressive changes in NH_3 adsorption behaviour and SCR activity as catalyst exposure time and temperature increase (Yao et al., 2023). Catalyst deactivation was found to correlate strongly with reductions in NH_3 storage capacity, highlighting the importance of maintaining accessible adsorption sites for sustained NO_x conversion.

Given these competing requirements, increasing attention has been directed towards multifunctional catalyst architectures. Combined SCR-ASC systems, layered catalyst designs, and hybrid Cu-Fe zeolite formulations have demonstrated potential to simultaneously achieve high NO_x conversion, low NH_3 slip, and reduced N_2O emissions over a broad operating window (Guan et al., 2014). Such integrated approaches are likely to play an important role in future NH_3-fuelled engine aftertreatment systems. Recent research has also increasingly focused on catalyst modification through promoter addition, hierarchical pore structures and tailored acidity to simultaneously improve low-temperature activity, hydrothermal stability and N_2 selectivity (Shi et al., 2023).

Overall, no single catalyst family currently satisfies all performance requirements associated with NH_3 combustion exhaust. Future catalyst development will therefore require a combination of improved material design, enhanced mechanistic understanding, and integrated optimisation of both combustion and aftertreatment systems.

4 Reaction mechanisms and kinetics

A fundamental understanding of reaction mechanisms and kinetics is essential for interpreting NH_3-SCR performance and developing reliable predictive models, particularly under the atypical conditions associated with NH_3-fuelled combustion. The SCR process comprises a complex network of adsorption, surface reactions, redox cycles, and competing side reactions that collectively determine catalyst activity, selectivity, and durability.

The activation of NH_3 is generally considered the initial and rate-determining step in both SCR and competing oxidation pathways. Following adsorption, NH_3 coordinates to Lewis acid sites or protonates on Brønsted acid sites depending on catalyst composition. Adsorbed NH_3 subsequently undergoes hydrogen abstraction to form surface amide (NH_2) species, which are widely recognised as key reactive intermediates. These NH_2 species react with NO to form unstable intermediates such as NH_2NO, which rapidly decompose to yield N_2 and H_2O. This sequence constitutes the basis of the standard SCR pathway and predominates when NO is the principal NO_x species present.

When both NO and NO_2 are available, the fast-SCR pathway becomes operative and substantially increases reaction rates, particularly at low temperatures. Fast SCR proceeds through interactions between adsorbed NH_3 species and oxidised NO_x intermediates, including nitrates and nitrites, resulting in more efficient conversion to N_2. Under NO_2-rich conditions, however, alternative pathways emerge. In particular, NH_4NO_3 can form and accumulate on catalyst surfaces at low temperatures. Subsequent decomposition of these deposits may generate N_2O, linking NO_2 chemistry directly to secondary GHG emissions. Such behaviour is especially relevant for NH_3-fuelled systems, where combustion conditions and upstream oxidation catalysts can significantly influence the NO:NO_2 ratio entering the SCR catalyst.

In parallel with NO_x reduction, several competing reactions consume NH_3 and influence overall selectivity. NH_3 oxidation becomes increasingly important at elevated temperatures or over highly oxidative catalyst formulations. Depending on catalyst composition and operating conditions, oxidation pathways may produce N_2, NO, or N_2O. The formation of N_2O is of particular concern because it can arise both from partial NH_3 oxidation and from the decomposition of NH_4NO_3 intermediates. In addition, imide (NH) species have been implicated in N_2O formation through reactions with NO, further increasing the complexity of the reaction network. Consequently, the dominant SCR pathway is strongly temperature dependent, requiring separate consideration of low-temperature SCR, standard SCR, fast SCR, and high-temperature NH_3 oxidation regimes in kinetic models (Wang et al., 2020).

4.1 Surface reaction mechanisms

At the mechanistic level, NH_3-SCR reactions are commonly described using three complementary frameworks: Langmuir–Hinshelwood (L–H), Eley–Rideal (E–R), and Mars–van Krevelen (MvK) mechanisms. In the L–H mechanism, both NH_3 and NO_x species adsorb on the catalyst surface prior to reaction, making this pathway particularly relevant for catalysts capable of NO oxidation and nitrate formation. In contrast, the E–R mechanism involves the direct reaction of gaseous NO with adsorbed NH_3-derived species such as NH_2, and is often invoked when NH_3 surface coverage is high or NO adsorption is relatively weak. For redox-active catalysts including vanadia systems and transition-metal-exchanged zeolites, the MvK mechanism provides an additional description in which lattice oxygen directly participates in oxidation reactions. During this process, metal centres such as V^{5+} or Cu^{2+} undergo cyclic reduction and reoxidation, with gaseous O_2 restoring the oxidised catalyst state.

Recent advances in operando spectroscopy, density functional theory (DFT), and microkinetic modelling have significantly refined understanding of these mechanisms. Studies on Cu-CHA catalysts indicate that catalytic activity is not governed solely by isolated Cu ions but also by dynamic multinuclear Cu species that form under

TABLE 5 Principal NH_3-SCR reaction mechanisms.

Mechanism	Description	Typical catalysts	Importance
Langmuir–hinshelwood (L-H)	Adsorbed NH_3 reacts with adsorbed NOx species	Zeolites, vanadia catalysts	Dominant at low-moderate temperatures
Eley-rideal (E-R)	Adsorbed NH_3 species react with gaseous NO	Cu-zeolites, Fe-zeolites	Important under NH_3-rich conditions
Mars-van krevelen (MvK)	Lattice O_2 participates directly in reaction	Vanadia, ceria, transition metal oxides	Governs redox cycles and NH_3 oxidation

reaction conditions. The mobility of these Cu centres facilitates oxygen activation and Cu^{2+}/Cu^{+} redox cycling, contributing to the exceptional low-temperature activity of Cu-zeolite catalysts (Paolucci et al., 2017). Furthermore, recent computational investigations suggest that E-R pathways involving gaseous NO reacting directly with adsorbed NH_2 species may contribute more substantially to overall SCR activity than previously recognised, particularly under NH_3-rich conditions typical of NH_3-fuelled exhaust streams (Voglar et al., 2023).

The coexistence of L-H, E-R, and MvK pathways presents a major challenge for kinetic model development. The dominant reaction route depends strongly on catalyst composition, temperature, NH_3 coverage, O_2 availability, and exhaust-gas composition. Consequently, predictive models must account for multiple parallel and competing pathways while remaining computationally tractable. From an emissions perspective, SCR performance is ultimately governed by the balance between desired NO_x reduction reactions and competing NH_3 oxidation pathways. Conditions that favour rapid NH_3 activation and selective NO_x reduction promote high N_2 selectivity, whereas excessive oxidation activity or accumulation of reactive intermediates increases the likelihood of undesirable by-products such as N_2O. Understanding these interactions remains essential for the design of catalysts and kinetic models tailored to NH_3-fuelled combustion systems. The principle ammonia-SCR reaction mechanisms are summarised in Table 5.

5 Modelling approaches for NH_3-SCR under ammonia combustion exhaust conditions

The development of predictive models for SCR systems has become increasingly important as NH_3-fuelled engines move from laboratory demonstrations toward practical deployment. Compared with conventional diesel exhaust, NH_3 combustion produces substantially different exhaust compositions, characterised by elevated NH_3 slip, variable NO_2 ratios, high water-vapour concentrations, and often lower exhaust gas temperatures (EGT). These factors introduce additional complexity into SCR modelling and require approaches capable of capturing both catalyst-scale reaction kinetics and system-level interactions between combustion and aftertreatment (Olsson et al., 2008).

A fundamental distinction between conventional urea-SCR systems and NH_3-fuelled engines lies in the origin of the reductant. In diesel applications, NH_3 generation from urea decomposition can be actively controlled to maintain the desired NH_3 ratio. In contrast, NH_3-fuelled engines generate NH_3 slip directly from the combustion process, causing reductant availability to vary with engine operating conditions. Consequently, future SCR models must explicitly account for the coupling between engine-out NH_3 production, catalyst utilisation, and downstream NO_x reduction performance.

5.1 Global kinetic models

Early SCR models were primarily based on global kinetic expressions derived from experimental reactor data. A major advance was the incorporation of dynamic NH_3 storage and adsorption kinetics, allowing transient catalyst behaviour during changing engine conditions to be represented more accurately (Nova et al., 2011). These models describe NO_x conversion using a limited number of lumped reactions representing standard SCR, fast SCR, and NH_3 oxidation pathways. Their relatively low computational cost makes them attractive for engine control applications and one-dimensional aftertreatment simulations (Koebel et al., 2000). However, because most were developed for conventional urea-SCR systems, they often struggle to accurately predict catalyst behaviour under NH_3-rich exhaust conditions, where surface coverage effects, NH_3 storage dynamics, and competing oxidation reactions become increasingly important.

5.2 Microkinetic and reactor-scale models

To improve mechanistic fidelity, researchers have developed microkinetic models that explicitly represent adsorption, desorption, surface reactions, and catalyst redox cycles. These models have proven particularly valuable for Cu- and Fe-exchanged zeolites, where SCR activity depends strongly on the oxidation state and mobility of active metal centres. Combined experimental and theoretical studies have demonstrated that Cu^{2+}/Cu^{+} redox cycling plays a central role in low-temperature SCR activity over Cu-CHA catalysts (Paolucci et al., 2017). Similarly, DFT and microkinetic investigations have provided detailed insights into the formation and consumption of nitrates, nitrites, and NH_2 intermediates, improving descriptions of both standard and fast SCR pathways. DFT studies further indicate that NH_3 activation proceeds differently on Brønsted and Lewis acid sites, highlighting the importance of catalyst acidity in determining SCR reaction pathways (Nova et al., 2009). DFT-derived microkinetic models provide valuable insight into the rate-limiting elementary reactions governing fast SCR, improving mechanistic understanding beyond conventional global kinetic models (Brüggemann et al., 2011).

Recent developments in chemical kinetic modelling have demonstrated that reduced reaction mechanisms can successfully reproduce SCR behaviour when key pathways, including standard

SCR, fast SCR, and NH_3 oxidation, are consistently parameterised (Burluka and Manning, 2025). However, these studies also highlight the strong sensitivity of SCR performance to NO oxidation, NH_3 storage, and the temperature-dependent competition between NO_x reduction and NH_3 oxidation. Under NH_3-fuelled engine conditions, where NH_3 slip and exhaust composition differ substantially from diesel exhaust, these sensitivities are expected to become even more pronounced, emphasising the need for revalidated kinetic frameworks.

5.3 Multi-scale and CFD modelling

At the reactor scale, one-dimensional and computational fluid dynamics (CFD) models are widely employed to describe the interaction between chemical kinetics and transport phenomena. These approaches couple reaction kinetics with heat transfer, species diffusion, and flow distribution within monolithic catalyst substrates. Reactor-scale simulations have shown that SCR reactions are often confined to a relatively thin near-surface region of the catalyst washcoat, whereas competing oxidation reactions can occur over a larger fraction of the catalyst wall. Such findings highlight the importance of accurately resolving washcoat diffusion, mass transfer limitations, and local temperature gradients. CFD studies have also demonstrated that catalyst geometry can significantly influence performance, with thin-walled monoliths and dual-layer catalyst architectures improving NH_3 utilisation and NO_x conversion while reducing undesired side reactions (Ogidiama, 2014).

Despite these advances, most reactor-scale studies have focused on conventional diesel aftertreatment systems. Similar transport-related challenges are expected under NH_3-fuelled engine conditions, where local variations in NH_3 slip may create regions of over- or under-stoichiometric catalyst operation, affecting both NO_x conversion and N_2O formation. Extending reactor-scale modelling frameworks to NH_3-rich exhaust environments therefore represents an important research priority.

More recently, multi-scale modelling frameworks have emerged that integrate combustion and aftertreatment processes within a single simulation environment. These approaches couple engine combustion models, which predict NO_x and NH_3 formation, with downstream catalyst models describing SCR performance (Song et al., 2015). Such integration is particularly important for NH_3-fuelled engines because exhaust composition depends strongly on combustion strategy, fuel substitution ratio, equivalence ratio, and engine load. Consequently, SCR performance cannot be accurately predicted without simultaneously considering combustion-generated NH_3 slip and NO_x formation.

5.4 Emerging data-driven approaches

Data-driven approaches are also gaining attention as complementary tools for catalyst modelling and control. Machine-learning techniques, including artificial neural networks, have demonstrated potential for predicting catalyst conversion efficiency, NH_3 slip, and emissions under varying operating conditions while significantly reducing computational cost (Liu et al., 2023). However, these methods remain dependent on large, high-quality experimental datasets and generally provide limited mechanistic insight. Hybrid frameworks that combine physically based kinetic models with data-driven optimisation may therefore offer the greatest potential for future NH_3-engine applications.

Although substantial progress has been achieved in global kinetics, microkinetic modelling, CFD simulations, and multi-scale frameworks, important limitations remain. Fully integrated modelling approaches capable of linking atomistic reaction chemistry, catalyst-scale processes, reactor transport phenomena, and engine operation remain relatively scarce (Lott and Deutschmann, 2023; Voglar et al., 2023). Furthermore, microkinetic models require large numbers of kinetic parameters and elementary reaction steps, many of which cannot be measured directly and must instead be estimated through parameter fitting. This introduces uncertainty when models are extrapolated beyond their calibration range.

Another significant limitation is the inadequate treatment of water adsorption and inhibition effects. Water vapour is one of the most abundant species in NH_3 and H_2 combustion exhaust, yet many SCR models continue to represent its influence using simplified competitive adsorption terms (Voglar et al., 2023). Recent hydrothermal ageing models have proposed active-site density as a physically meaningful descriptor of catalyst degradation, linking activity loss directly to changes in Brønsted and Lewis acid site populations during ageing (Yao et al., 2023). Dual-site kinetic models accounting separately for Brønsted and Lewis acid sites have demonstrated improved capability for predicting catalyst behaviour following hydrothermal exposure. Theoretical studies further suggest that water can influence proton-transfer processes and NH_3 adsorption equilibria beyond simple site competition, indicating that current representations may underestimate its impact on SCR kinetics (Nova et al., 2009).

Accurate prediction of N_2O formation remains an additional challenge. N_2O production involves multiple competing pathways, including NH_3 oxidation, NH_4NO_3 formation and decomposition, and catalyst-specific surface reactions, making reliable prediction difficult across a wide operating window (Jung et al., 2022). Transient operating conditions, catalyst ageing, and interactions between combustion and aftertreatment systems introduce further uncertainty.

Overall, SCR modelling capabilities have advanced considerably over the past 2 decades, yet most existing frameworks remain rooted in diesel-derived exhaust conditions. Future modelling efforts should focus on experimentally validated, multi-scale approaches capable of capturing NH_3-rich exhaust chemistry, catalyst ageing, water inhibition effects, and N_2O formation pathways under realistic NH_3-combustion conditions. Such models will be essential for optimising catalyst design, reducing NH_3 slip, mitigating N_2O emissions, and enabling efficient operation of next-generation NH_3-fuelled power and propulsion systems. A comparison of SCR modelling approaches is provided in Table 6.

6 Experimental advances in NH_3-SCR for ammonia combustion exhaust

Experimental investigations have played a central role in advancing SCR technology for NH_3-fuelled engines by providing the validation required for catalyst development, mechanistic

TABLE 6 Comparison of SCR modelling approaches.

Modelling approach	Characteristics	Advantages	Limitations
Microkinetic	Elementary reaction network	Mechanistic insight	Large parameter requirements
Global kinetics	Lumped reactions	Computationally efficient	Limited predictive capability
1-D reactor models	Axial transport and kinetics	Fast simulation	Limited spatial resolution
CFD models	Detailed flow, heat and mass transfer	High fidelity	Computationally expensive
Multi-scale models	Combustion + aftertreatment coupling	System-level optimisation	High complexity
Machine learning	Data-driven prediction	Rapid computation	Limited physical interpretability

understanding, and kinetic model formulation. Compared with conventional diesel exhaust, NH_3 combustion generates exhaust streams characterised by elevated NH_3 slip, variable NO:NO_2 ratios, and lower exhaust gas temperatures (EGT), all of which influence catalyst activity, selectivity, and durability (Lesmana et al., 2021; Valera-Medina et al., 2018). As a result, significant research effort has focused on evaluating the suitability of existing SCR catalyst technologies under NH_3-rich conditions.

Early studies primarily examined conventional catalyst families, including vanadia-based systems and transition-metal-exchanged zeolites. Commercial V_2O_5-WO_3/TiO_2 catalysts demonstrated high NO_x conversion efficiencies and excellent N_2 selectivity within their optimal operating window of approximately 300 °C–450 °C, although activity declined substantially at lower temperatures and NH_3 oxidation became increasingly significant at elevated temperatures (Koebel et al., 2000; Nova et al., 2009). Subsequent investigations of Cu- and Fe-exchanged zeolites revealed markedly improved low-temperature performance, with Cu-CHA catalysts achieving near-complete NO_x conversion below 250 °C under fast-SCR conditions (Gao et al., 2013). However, this enhanced activity is often accompanied by increased NH_3 oxidation and N_2O formation under NH_3-rich conditions when compared with vanadia-based catalysts (Jung et al., 2022).

Consequently, experimental catalyst development has increasingly focused on improving low-temperature activity while maintaining high N_2 selectivity and minimising N_2O formation. For Cu-CHA catalysts, spectroscopic and kinetic studies have shown that catalytic performance depends strongly on the distribution, mobility, and redox behaviour of Cu ions within the zeolite framework (Paolucci et al., 2017). Optimisation of copper loading and framework composition has been shown to improve NH_3 storage capacity and low-temperature activity while suppressing undesirable oxidation pathways. Similarly, Fe-exchanged zeolites (FeZ) have attracted considerable attention for high-temperature applications owing to their superior thermal stability and resistance to hydrothermal ageing compared with Cu-based catalysts (Brandenberger et al., 2008).

6.1 Influence of operating conditions

Beyond catalyst formulation, reactor-scale studies have provided valuable insight into the influence of operating conditions on SCR performance. Temperature, gas hourly space velocity (GHSV), O_2 concentration, and feed composition have all been shown to strongly affect NO_x conversion efficiency and selectivity. Among these variables, the NO_2:NO_x ratio is particularly important because approximately equimolar concentrations of NO and NO_2 promote the fast-SCR pathway and substantially enhance low-temperature activity (Song et al., 2015). This finding is especially relevant for ammonia-fuelled engines, where combustion conditions and upstream oxidation processes can significantly alter NO:NO_2 speciation entering the catalyst.

Transient reactor studies have further highlighted the importance of NH_3 storage and release phenomena. Temperature-programmed desorption (TPD), concentration step-change experiments, and transient response analyses have demonstrated that catalyst NH_3 storage capacity (NSC) strongly influences performance during dynamic operation (Nova et al., 2011; Olsson et al., 2008). While increased NH_3 storage can sustain NO_x conversion during temporary fluctuations in reductant availability, it may also lead to delayed NH_3 breakthrough and increased NH_3 slip. These effects are particularly important in NH_3-fuelled systems, where NH_3 simultaneously acts as the fuel, pollutant, and SCR reductant.

6.2 Engine-based and integrated aftertreatment studies

More recently, experimental research has increasingly shifted from laboratory-scale reactors towards integrated engine-aftertreatment investigations. Studies on NH_3 and NH_3-diesel DF engines have demonstrated the feasibility of utilising engine-out NH_3 slip as a reductant for downstream SCR reactions (Cardoso et al., 2021; Lesmana et al., 2021). These investigations confirmed that passive utilisation of NH_3 slip can significantly reduce external urea demand; however, the naturally occurring NH_3:NO_x ratio often varies substantially with engine operating condition and is frequently insufficient to achieve complete NO_x removal across the full operating range. Consequently, supplementary NH_3 dosing, combustion optimisation, or alternative control strategies may still be required to achieve near-zero emissions.

Alongside NO_x conversion, the environmental significance of N_2O emissions has received increasing attention. Experimental studies have shown that N_2O formation depends strongly on catalyst composition, temperature, and NO_2 concentration (Jung et al., 2022). Excessive NO_2 promotes the formation of NH_4NO_3 species, which subsequently decompose to produce N_2O at

intermediate temperatures. Comparative catalyst evaluations have further demonstrated that Cu-zeolites generally exhibit higher N_2O formation tendencies than vanadia-based catalysts, while Fe-zeolites display intermediate behaviour depending on operating conditions. These findings highlight the need to evaluate catalyst performance using both NO_x conversion efficiency and N_2O selectivity, particularly for NH_3-fuelled applications where NH_3-rich conditions are common.

Advances in characterisation techniques have significantly improved mechanistic understanding of SCR catalysts and reaction pathways. *In situ* diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS), X-ray absorption spectroscopy (XAS), and operando spectroscopic techniques have enabled direct observation of adsorbed NH_3 species, nitrates, nitrites, and catalyst redox transitions during operation (Paolucci et al., 2017). These studies have provided experimental evidence supporting both L-H and E-R reaction pathways and have played an important role in validating modern microkinetic models.

Despite substantial progress, several experimental challenges remain. Most published studies continue to use simplified synthetic gas mixtures that do not fully replicate the complexity of NH_3-combustion exhaust. Long-term investigations examining the combined effects of high NH_3 concentrations, water vapour, sulphur species, and thermal cycling remain relatively scarce. Furthermore, the interactions between SCR and ASC catalysts, and upstream oxidation catalysts under realistic operating conditions are still not fully understood.

Overall, experimental research has established the technical feasibility of SCR for NH_3-fuelled engines while providing critical insight into catalyst activity, selectivity, reaction mechanisms, and durability. However, further integrated engine-scale investigations, transient studies, and long-term ageing assessments are required to optimise catalyst systems for practical NH_3-combustion applications and to balance NO_x reduction with control of NH_3 slip and N_2O emissions.

7 Coupling between combustion and aftertreatment

The performance of SCR systems in NH_3-fuelled engines is intrinsically linked to upstream combustion processes. Unlike conventional diesel engines, where NH_3 availability can be independently regulated through urea dosing, NH_3-fuelled systems generate both NO_x and NH_3 slip directly from combustion. Consequently, the composition of the exhaust entering the catalyst is determined by engine operating conditions, creating a strong interdependence between combustion and aftertreatment performance (Cardoso et al., 2021; Lesmana et al., 2021).

Among the combustion parameters influencing SCR operation, engine load, combustion phasing, and equivalence ratio exert the greatest effect on exhaust composition. Experimental studies on NH_3-fuelled spark-ignition (SI) and compression-ignition (CI) engines have shown that low-load operation generally produces higher NH_3 slip because of incomplete fuel conversion, while NO_x emissions remain comparatively low due to reduced combustion temperatures (Kobayashi et al., 2019; Valera-Medina et al., 2018). As load increases, improved combustion efficiency reduces NH_3 slip, but higher in-cylinder temperatures promote fuel-NO formation, resulting in increased NO_x emissions. This inverse relationship complicates maintenance of the optimum NH_3:NO_x ratio required for efficient SCR operation.

The equivalence ratio has a similarly important influence. Lean combustion promotes oxidation of fuel-bound nitrogen species and favours NO formation, whereas richer conditions suppress NO_x production but increase emissions of unburned NH_3 and other partially oxidised species (Otomo et al., 2018). Experimental investigations by Lesmana et al., 2019 demonstrated that engine-out NH_3 concentrations vary substantially with equivalence ratio (ϕ) and are frequently insufficient to achieve complete NO_x conversion without supplementary reductant supply. These observations suggest that passive utilisation of NH_3 slip as the sole SCR reductant may only be feasible over limited operating regions.

H_2-assisted NH_3 combustion introduces additional interactions between combustion and aftertreatment systems. H_2 enrichment improves combustion stability, accelerates flame propagation, and enhances NH_3 conversion efficiency, thereby reducing NH_3 slip and extending lean operating limits (Lhuillier et al., 2020). However, the increased concentrations of reactive radicals such as O, OH, and HO_2 can alter NO oxidation chemistry and influence the NO:NO_2 ratio entering the catalyst. Liu et al., 2011 reported that residual H_2 in the exhaust can promote NO oxidation to NO_2, potentially enhancing low-temperature fast-SCR activity. H_2 addition also increases exhaust water vapour concentrations, which may further influence downstream catalyst performance through competitive adsorption and changes in reaction kinetics. Consequently, optimisation of NH_3-H_2 combustion strategies should consider aftertreatment performance in addition to combustion efficiency and stability.

7.1 NH_3-NO_x ratio and catalyst performance

The NH_3:NO_x ratio at the SCR inlet remains the most important parameter governing catalyst performance. Standard SCR chemistry requires approximately equimolar quantities of NH_3 and NO_x for complete conversion, whereas deviations from this ratio either limit NO_x reduction or increase NH_3 slip (Koebel et al., 2000). In NH_3-fuelled engines, however, this ratio is controlled primarily by combustion behaviour rather than external dosing systems. Although (Cardoso et al., 2021) proposed that engine-out NH_3 slip could potentially eliminate the need for urea injection, experimental studies indicate that substantial fluctuations in NH_3:NO_x ratio occur during load changes and transient operation (Lesmana et al., 2021). Furthermore, while increasing NH_3 availability generally improves NO_x conversion, excessive NH_3 can promote NH_3 oxidation and N_2O formation, highlighting the need for careful management of reductant availability (Wu et al., 2024).

Thermal coupling between the engine and catalyst system is equally important. NH_3 combustion frequently produces lower exhaust gas temperatures (EGT) than conventional diesel combustion, particularly under lean and low-load conditions (Valera-Medina et al., 2018). These temperatures may fall below the optimal operating window of many SCR catalysts, reducing NH_3

activation rates and limiting NO_x conversion efficiency. Conversely, high-load operation can expose catalysts to temperatures at which NH_3 oxidation and N_2O formation become increasingly significant (Jung et al., 2022). As a result, catalyst performance cannot be considered independently of the thermal characteristics of the combustion process.

7.2 Integrated combustion-aftertreatment optimisation

The strong coupling between combustion and aftertreatment extends beyond NH_3 slip and NO_x emissions to include GHG formation. Improvements in combustion efficiency can simultaneously reduce NH_3 slip and engine-out N_2O emissions, thereby lowering the burden placed on downstream catalysts (Pedersen et al., 2023). demonstrated that controlling combustion-generated NH_3 and N_2O is as important as catalyst optimisation when minimising overall emissions from NH_3-fuelled engines.

Recognising these interactions, recent modelling studies have increasingly adopted integrated engine-aftertreatment frameworks that simultaneously predict combustion emissions, NH_3 slip, catalyst NO_x conversion efficiency, and secondary pollutant formation (Zhang et al., 2023; Gopinathan and Mohamed Ibrahim, 2025). These coupled approaches enable optimisation of combustion parameters and catalyst operation at the system level rather than treating them as separate subsystems. Such integration is particularly important for NH_3-fuelled engines because NH_3 functions simultaneously as the fuel, pollutant, and SCR reductant.

Figure 2 illustrates the coupling between combustion and aftertreatment in NH_3-fuelled engines. Engine operating conditions govern the formation of NO_x, NH_3 slip, H_2O, and N_2O, which determine the inlet conditions to the SCR catalyst. In turn, catalyst performance depends on these engine-out species and influences the overall emissions released to the atmosphere.

Overall, available evidence demonstrates that SCR performance in NH_3-fuelled engines cannot be optimised independently of combustion. Exhaust composition, temperature, NH_3 slip, NO_x speciation, and N_2O formation are all strongly governed by combustion behaviour, while catalyst performance in turn influences overall emissions. Future developments are therefore likely to focus on integrated combustion–aftertreatment optimisation, where engine calibration, catalyst selection, and emissions control are treated as components of a single interconnected system.

8 N_2O formation and mitigation strategies

Nitrous oxide (N_2O) is emerging as one of the principal environmental challenges associated with NH_3-fuelled combustion systems because reductions in NO_x emissions may be accompanied by increases in greenhouse-gas emissions. With a global warming potential approximately 273 times greater than that of CO_2 over a 100-year time horizon, even relatively small quantities of N_2O can significantly affect the overall environmental performance of

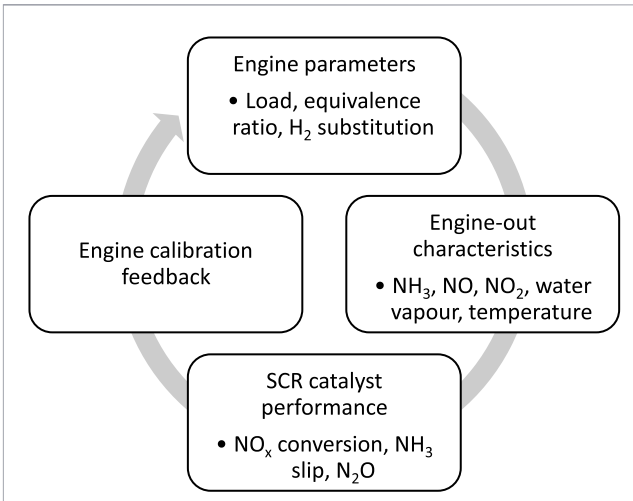


FIGURE 2
Schematic illustration of combustion–aftertreatment coupling in NH_3-fuelled engine emission control systems.

NH_3-fuelled engines. Although NH_3 combustion generally produces limited engine-out N_2O because of the high combustion temperatures involved, substantial quantities can be generated within SCR and NH_3 oxidation catalysts as undesired by-products of NO_x abatement reactions (Guan et al., 2014; Jung et al., 2022). Consequently, minimising N_2O emissions has become an increasingly important objective in the development of aftertreatment systems for NH_3-fuelled applications.

N_2O formation within NH_3-SCR systems is generally attributed to two principal pathways. The first involves partial oxidation of NH_3, which becomes increasingly important at elevated temperatures and on highly oxidative catalyst surfaces. Depending on catalyst composition and operating conditions, NH_3 oxidation proceeds through reactive intermediates such as NH_2 and NH species and may ultimately produce N_2, NO, or N_2O. Excess NH_3 concentrations and high oxygen availability generally favour N_2O formation through these pathways (Ramis et al., 1996).

The second major pathway involves the formation and decomposition of NH_4NO_3. Under low-temperature and NO_2-rich conditions, NH_3 reacts with NO_2 to form surface ammonium nitrate species that accumulate within catalyst pores. As temperature increases, these species become unstable and decompose, generating N_2O and water vapour (Madia et al., 2002). This mechanism is particularly important during fast-SCR operation and under conditions where local NO_2 concentrations exceed the optimum NO_2:NO_x ratio. Accordingly, NH_4NO_3 should be regarded not merely as a catalyst deposit but as a key low-temperature SCR intermediate that strongly influences NO_x conversion, NH_3 storage behaviour, and N_2O formation.

8.1 Influence of catalyst composition and operating conditions

The relative importance of these pathways depends strongly on catalyst composition and operating temperature. Comparative

studies of commercial SCR catalysts have demonstrated substantial differences in N_2O selectivity. Vanadia-based catalysts generally exhibit relatively low N_2O formation across a broad operating window because of their balanced acid-redox properties and moderate NH_3 oxidation activity. In contrast, Cu-exchanged zeolites, although highly active for low-temperature NO_x reduction, can generate significant quantities of N_2O under NH_3-rich conditions and during NH_3 oxidation reactions (Paolucci et al., 2017). Fe-zeolite (FeZ) catalysts often exhibit lower low-temperature activity but may promote N_2O formation at elevated temperatures where NH_3 oxidation becomes increasingly significant. Experimental work by (Jung et al., 2022) further demonstrated that Fe-zeolite catalysts initiated N_2O formation earlier than Cu-zeolites owing to differences in NO depletion and NO_2 consumption pathways.

Temperature exerts a particularly complex influence on N_2O selectivity. At temperatures below approximately 250 °C, N_2O formation is dominated by NH_4NO_3 chemistry and incomplete SCR reactions. As catalyst temperature increases, decomposition of stored NH_4NO_3 can generate transient N_2O emission peaks. At higher temperatures, typically above 350 °C–400 °C, NH_3 oxidation becomes the dominant source of N_2O, especially in the presence of excess NH_3 or highly oxidative catalyst formulations (Jung et al., 2022). This dual temperature dependence complicates catalyst optimisation because strategies designed to suppress low-temperature N_2O formation may inadvertently increase high-temperature NH_3 oxidation activity.

8.2 Strategies for N_2O mitigation

Consequently, N_2O mitigation requires both catalyst-level and system-level approaches. Catalyst development efforts increasingly focus on formulations that maximise NO_x reduction to N_2 while suppressing competing NH_3 oxidation pathways. Adjustments to active metal loading, promoter composition, and catalyst acidity have been shown to improve N_2 selectivity while maintaining high $deNO_x$ activity (Damma et al., 2019; Paolucci et al., 2017). Hybrid catalyst architectures incorporating SCR catalysts with downstream ammonia slip catalysts (ASC) have also been investigated as a means of controlling NH_3 emissions while limiting secondary N_2O formation.

Operational control is equally important. Maintaining the NH_3:NO_x ratio close to unity minimises excess NH_3 available for oxidation, while controlling the NO_2:NO_x ratio limits ammonium nitrate formation (Song et al., 2015). Thermal management through catalyst placement, insulation, and exhaust heat recovery can further reduce residence within temperature windows that favour N_2O generation. For NH_3-fuelled engines, these strategies must be considered alongside combustion optimisation because both NH_3 slip and NO_x formation originate directly from the combustion process.

Recent studies have also demonstrated that catalyst ageing can significantly influence N_2O behaviour. Hydrothermal ageing alters not only catalyst activity but also the temperature window and selectivity for N_2O formation (Liu et al., 2023). reported that ageing shifts N_2O formation towards higher temperatures and modifies the catalyst's inhibitory effect on N_2O production. These findings suggest that optimisation based solely on NO_x conversion efficiency may be insufficient, as catalysts exhibiting superior $deNO_x$ performance do not necessarily minimise N_2O emissions (Jung et al., 2022).

Beyond conventional SCR optimisation, direct catalytic decomposition of N_2O has emerged as a promising supplementary mitigation strategy. Fe-containing zeolites and transition-metal-exchanged catalysts have demonstrated significant N_2O decomposition activity between approximately 400 °C and 600 °C, converting N_2O directly to N_2 and O_2 (Zhuang et al., 2024). Such materials could potentially be integrated into future NH_3-engine aftertreatment architectures to provide simultaneous control of NO_x, NH_3 slip, and N_2O emissions. An additional advantage is that many N_2O decomposition catalysts are inhibited by excess O_2 because it competes for active sites and limits catalyst regeneration. While this represents a challenge in O_2-rich diesel exhaust, the lower O_2 concentrations often encountered in NH_3-fuelled engine exhaust may create more favourable conditions for N_2O decomposition. This raises the possibility of integrated catalyst systems capable of simultaneously achieving $deNO_x$ performance and GHG mitigation.

Overall, N_2O mitigation is becoming a critical design objective for NH_3-fuelled engine aftertreatment systems. Future catalyst development must balance NO_x conversion efficiency, NH_3 slip control, catalyst durability, and N_2O selectivity simultaneously. Achieving this objective will require improved mechanistic understanding of N_2O formation pathways, optimisation of catalyst formulations, and closer integration of combustion and aftertreatment strategies under realistic NH_3-rich exhaust conditions. The major Nitrous oxide formation pathways and mitigation strategies are summarised in Table 7.

9 Challenges and research gaps

A number of important challenges remain before NH_3-SCR systems can be fully optimised for NH_3-fuelled combustion applications. Although substantial progress has been made in catalyst development, reaction mechanism identification, and numerical modelling, many existing studies remain focused on conventional diesel-derived exhaust compositions rather than the NH_3-rich environments characteristic of NH_3 combustion (Lesmana et al., 2021; Valera-Medina et al., 2018).

One of the most significant limitations is the lack of integrated experimental and modelling studies. Detailed reaction mechanisms have been developed using laboratory reactors, spectroscopic techniques, and density functional theory, while increasingly sophisticated kinetic and reactor-scale models have been proposed (Paolucci et al., 2017). However, relatively few investigations have combined mechanistic modelling with validation under realistic NH_3-engine operating conditions. Consequently, many existing models remain catalyst-specific and cannot be readily transferred across catalyst formulations, exhaust compositions, or operating regimes.

9.1 Experimental and modelling challenges

The availability of representative experimental data also remains limited. Most SCR performance maps, kinetic parameters, and

TABLE 7 Major N_2O formation pathways and mitigation strategies.

N_2O formation pathway	Reactions	Conditions favouring formation	Mitigation strategy
Partial NH_3 oxidation	$2NH_3 + 2O_2 \rightarrow N_2O + 3H_2O$	High temperature (350–400 °C), excess NH_3, Cu-zeolites > Fe-zeolites > V-based	Improve catalyst selectivity and redox properties, optimise NH_3:NOx ratio
NH_4NO_3 formation and decomposition	$NH_3 + HNO_3 \rightleftharpoons NH_4NO_3(s)$ $NH_4NO_3 \rightarrow N_2O + 2H_2O$	Low temperature (150 °C), NO_2-rich conditions	Minimise NO_2 excess (maintain NO_2:$NO_x \approx 0.5$), avoid low-temperature operation
NH_2NO intermediate decomposition	$NH_2 + NO \rightarrow NH_2NO$ $NH_2NO \rightarrow N_2O + H_2$	Intermediate temperature (mechanism dependent)	Promote selective SCR pathways that favour direct N_2 formation
NH intermediates reacting with NO	$NH + NO \rightarrow N_2O + H$	NH_3-rich environments, favoured by highly oxidative catalysts	Tailored active-site design, reduce formation of NH radicals by limiting excessive NH_3 oxidation
NH_3 oxidation over ASC	$2NH_3 + 2O_2 \rightarrow N_2O + 3H_2O$	Excess NH_3 downstream	Optimised ASC formulation
Hydrothermal aging effects	Ageing alters NH_3 oxidation and SCR pathways, increasing N_2O selectivity	Catalyst lifetime dependent	Improve hydrothermal stability and maintain active site density

model validation datasets have been generated using synthetic gas mixtures designed to emulate diesel exhaust. NH_3-fuelled engines, however, produce exhaust streams containing elevated NH_3 slip, altered NO:NO_2 ratios, lower O_2 concentrations, and high water-vapour contents. These differences may substantially influence catalyst activity, selectivity, and durability, highlighting the need for dedicated experimental studies under realistic NH_3-combustion conditions.

At the reactor and system scales, modelling capabilities remain underdeveloped for NH_3-fuelled applications. While detailed CFD frameworks coupling transport phenomena with SCR kinetics have been successfully applied to urea-SCR systems, their extension to NH_3-fuelled engines remains limited (Guo Y, 2017). Future models should explicitly incorporate engine-out NH_3 slip, coupled oxidation-reduction chemistry, NH_3 storage dynamics, and N_2O formation pathways to enable accurate prediction of catalyst performance under NH_3-rich exhaust conditions. Similarly, integrated combustion-aftertreatment models are required to capture the strong coupling between combustion-generated NH_3, NO_x formation, and downstream catalyst behaviour.

A major unresolved issue concerns the formation of N_2O. Although several pathways have been proposed, including NH_3 oxidation, NH_2NO intermediates, and NH_4NO_3 formation and decomposition, their relative contributions remain highly dependent on catalyst composition and operating conditions. This uncertainty limits both catalyst optimisation and predictive modelling, particularly because catalysts exhibiting excellent NO_x conversion do not necessarily minimise N_2O emissions. Improved mechanistic understanding of N_2O formation under NH_3-rich conditions therefore remains a critical research priority.

Transient operation represents another important knowledge gap. Most experimental studies and model validations are performed under steady-state conditions, whereas practical engines experience continual fluctuations in load, temperature, and exhaust composition. Under such conditions, NH_3 storage and release dynamics can strongly influence NO_x conversion, NH_3 slip, and N_2O formation (Olsson et al., 2008; Song et al., 2015). Developing transiently validated kinetic models and conducting dynamic engine-scale experiments will therefore be essential for future system optimisation.

9.2 Catalyst durability and ageing

Long-term catalyst durability also requires further investigation. NH_3-fuelled engines expose catalysts to prolonged NH_3-rich atmospheres, high water-vapour concentrations, and, in DF applications, potential contaminants originating from pilot fuels. These conditions may accelerate hydrothermal degradation, active-site migration, sulphation, and zeolite framework deterioration (Paolucci et al., 2017). In addition to reducing catalyst activity, ageing may alter reaction pathways and catalyst selectivity, potentially affecting NH_3 slip and N_2O formation. Recent studies further suggest that water adsorption plays a more significant role in SCR kinetics than is currently represented in most models, particularly given the high water-vapour concentrations present in NH_3-combustion exhaust (Voglar et al., 2023).

Finally, there remains a need for catalyst formulations specifically tailored to NH_3-fuelled exhaust environments. Current commercial SCR catalysts were largely developed for diesel applications and may not be optimised for sustained exposure to elevated NH_3 concentrations, H_2 co-firing, reduced O_2 availability, or the unique emissions characteristics of NH_3 combustion. Future catalyst development should therefore adopt a multi-objective approach that simultaneously considers NO_x conversion, NH_3 slip, N_2O mitigation, catalyst durability, and overall GHG performance.

Overall, future progress will require closer integration of catalyst design, combustion development, experimental validation, and multi-scale modelling. Addressing these challenges will be essential for enabling SCR systems capable of delivering effective NO_x control while minimising NH_3 slip and N_2O emissions in next-generation NH_3-fuelled power and propulsion systems. Current research gaps and future needs for ammonia combustion exhaust treatment are summarised in Table 8.

TABLE 8 Current research gaps and future needs for treatment of ammonia combustion exhaust.

Research area	Current limitation	Future requirement
Catalyst development	No catalyst optimised specifically for NH_3-rich exhaust	Tailored NH_3-combustion catalysts
N_2O prediction	Poor mechanistic understanding	Detailed kinetic studies
Modelling	Mostly developed for diesel SCR	NH_3-specific models
Transient operation	Limited engine-cycle data	Dynamic experimental validation
Durability	Lack of long-term studies	Aging and poisoning investigations
AI integration	Limited implementation	Data-driven catalyst optimisation

10 Future research directions

The application of SCR technology to NH_3-fuelled combustion presents challenges that extend beyond those encountered in conventional diesel aftertreatment systems. The simultaneous presence of NH_3 slip, variable NO_x speciation, high water-vapour concentrations, and fluctuating exhaust temperatures creates a highly dynamic reaction environment that requires both catalyst innovation and improved system integration. Unlike conventional urea-SCR systems, where reductant dosing can be independently controlled, NH_3-fuelled engines generate both NO_x and NH_3 slip directly from the combustion process, creating a strong coupling between combustion behaviour and catalyst performance.

A key opportunity offered by NH_3-fuelled engines is the potential utilisation of engine-out NH_3 slip as the reductant for downstream SCR reactions. In principle, this could eliminate the need for external urea infrastructure and simplify aftertreatment system design (Kobayashi et al., 2019; Kuta et al., 2023). However, experimental studies have demonstrated that the NH_3:NO_x ratio varies significantly with engine operating conditions, often resulting in either insufficient NH_3 for complete NO_x conversion or excessive NH_3 slip that promotes secondary emissions. Effective utilisation of combustion-generated NH_3 therefore remains a major challenge requiring coordinated optimisation of both engine operation and catalyst performance.

Current SCR catalyst technologies each offer distinct advantages and limitations under NH_3-combustion conditions. Cu-exchanged zeolites provide excellent low-temperature activity and high NH_3 storage capacity but may exhibit increased N_2O formation under NH_3-rich conditions. Fe-zeolites offer superior thermal stability and favourable high-temperature performance, while vanadia-based catalysts remain highly selective for NO_x reduction but are constrained by narrower operating windows and long-term durability concerns (Paolucci et al., 2017). These limitations have stimulated growing interest in catalyst formulations specifically tailored to NH_3-rich exhaust environments.

Consequently, future catalyst development is increasingly focused on multifunctional and hybrid catalyst architectures. Layered Cu-Fe zeolite systems, combined SCR-ammonia slip catalyst (ASC) configurations, and catalysts engineered to suppress NH_3 oxidation are being explored to broaden operating windows and improve selectivity. Beyond conventional SCR optimisation, there is growing interest in integrating dedicated N_2O decomposition functionality within aftertreatment systems. Multifunctional catalyst platforms capable of simultaneously reducing NO_x, utilising NH_3 slip, and decomposing N_2O could provide a pathway toward near-zero emissions from NH_3-fuelled engines.

Advances in modelling are expected to play a critical role in accelerating catalyst and system development. Significant progress has been achieved through density functional theory (DFT), microkinetic modelling, and multi-scale simulation frameworks; however, predictive capability remains limited under realistic NH_3-engine conditions. Improved integration of atomistic reaction energetics, operando spectroscopy, microkinetic models, and reactor-scale simulations offers considerable potential for improving mechanistic understanding and reducing uncertainty in model parameters (Paolucci et al., 2017; Voglar et al., 2023). At the same time, machine-learning-assisted catalyst design and data-driven optimisation methods may help accelerate catalyst screening and reduce experimental costs.

Future developments will likely require a shift from isolated catalyst optimisation toward integrated combustion-aftertreatment design. SCR performance cannot be optimised independently because combustion conditions directly determine catalyst inlet temperature, NH_3 availability, NO_x concentration, and exhaust composition. Consequently, future NH_3-engine systems will require coordinated control of combustion phasing, fuel substitution ratio, exhaust thermal management, NH_3 slip utilisation, and catalyst operation. Integrated modelling and control frameworks capable of simultaneously optimising combustion and aftertreatment performance are therefore expected to become increasingly important. Future aftertreatment development is expected to move towards integrated catalyst-system optimisation, combining heterogeneous reaction engineering with advanced modelling and control strategies (Lott and Deutschmann, 2023).

A further priority is the generation of representative experimental datasets for model validation and catalyst assessment. Long-duration engine testing, transient operating cycles, hydrothermal ageing studies, and experiments using realistic NH_3-combustion exhaust compositions remain comparatively scarce. In particular, greater attention should be given to the effects of high water-vapour concentrations, NH_3-rich operating conditions, catalyst ageing, and transient operation, as these factors are expected to strongly influence catalyst activity, selectivity, and durability.

Ultimately, future research must move beyond maximising NO_x conversion alone and instead pursue holistic optimisation of emissions performance. Achieving this objective will require

coordinated advances in catalyst science, reaction engineering, combustion development, control systems, and predictive modelling. The successful integration of these disciplines will be essential for developing NH_3-fuelled power and propulsion systems capable of simultaneously minimising NO_x, NH_3 slip, and N_2O emissions while maintaining long-term catalyst durability and operational efficiency.

11 Conclusion

NH_3 is increasingly recognised as a promising carbon-free fuel for future transportation and power-generation systems. However, the successful deployment of NH_3-fuelled engines depends on effective control of NO_x emissions and unburned NH_3, making SCR technology a critical component of future exhaust aftertreatment systems.

This review has examined the unique characteristics of NH_3 combustion exhaust and their implications for SCR performance. Compared with conventional diesel exhaust, NH_3-fuelled systems present substantially different operating conditions, including elevated NH_3 slip, variable $NO{:}NO_2$ ratios, lower exhaust temperatures, and an increased risk of N_2O formation. Together, these factors strongly influence catalyst activity, selectivity, and durability.

A review of catalyst technologies highlights that no single catalyst family currently satisfies all performance requirements. Cu-exchanged zeolites offer excellent low-temperature activity, Fe-zeolites provide superior high-temperature stability, and vanadia-based catalysts remain highly selective within intermediate temperature ranges. Consequently, increasing attention is being directed towards hybrid catalyst architectures that combine the advantages of multiple catalyst systems while mitigating their individual limitations.

The mechanistic complexity of NH_3-SCR reactions presents significant challenges for both catalyst design and predictive modelling. Multiple reaction pathways, including standard SCR, fast SCR, NH_3 oxidation, ammonium nitrate chemistry, and N_2O formation, operate simultaneously and are strongly influenced by catalyst composition and operating conditions. Although substantial progress has been made in kinetic modelling, further development is required to accurately predict catalyst behaviour under realistic NH_3-combustion conditions.

Experimental investigations have provided valuable insights into catalyst performance, reaction mechanisms, and system integration. However, important gaps remain regarding transient operation, catalyst ageing, water-vapour effects, and N_2O selectivity under NH_3-rich exhaust environments. Furthermore, the strong coupling between combustion and aftertreatment emphasises the need for integrated optimisation approaches that consider engine operation and catalyst performance simultaneously.

A central conclusion emerging from this review is that NH_3-fuelled engines fundamentally alter the operating environment of SCR systems. Elevated NH_3 slip, high water-vapour concentrations, altered NO_x speciation, and the growing importance of N_2O emissions challenge many of the assumptions established for conventional diesel aftertreatment. As a result, catalyst development, kinetic modelling, combustion optimisation, and emissions-control strategies can no longer be considered independently. Future progress will depend on the development of catalyst systems specifically tailored to NH_3-combustion exhaust, supported by realistic experimental validation and integrated multi-scale modelling frameworks. Achieving robust control of NO_x, NH_3 slip, and N_2O emissions will be essential for realising the full potential of NH_3 as a sustainable fuel for next-generation power and propulsion systems.

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References

Abu-Jrai, A. M., Al-Muhtaseb, A. H., and Hasan, A. O. (2017). Combustion, performance, and selective catalytic reduction of NOx for a diesel engine operated with combined tri fuel (H2, CH4, and conventional diesel). *Energy* 119, 901–910. doi: 10.1016/j.energy.2016.11.050

Borfecchia, E., Lomachenko, K. A., Giordanino, F., Falsig, H., Beato, P., Soldatov, A. V., et al. (2015). Revisiting the nature of Cu sites in the activated Cu-SSZ-13 catalyst for SCR reaction. *Chem. Sci.* 6 (1), 548–563. doi: 10.1039/C4SC02907K

Brandenberger, S., Kröcher, O., Tissler, A., and Althoff, R. (2008). The state of the art in selective catalytic reduction of NO_x by ammonia using metal-exchanged zeolite catalysts. *Catal. Rev.* 50 (4), 492–531. doi: 10.1080/01614940802480122

Brüggemann, T. C., Vlachos, D. G., and Keil, F. J. (2011). Microkinetic modeling of the fast selective catalytic reduction of nitrogen oxide with ammonia on H-ZSM5 based on first principles. *J. Catal.* 283 (2), 178–191. doi: 10.1016/j.jcat.2011.08.009

Burluka, A. A., and Manning, A. P. (2025). Chemical kinetic mechanism for selective catalytic reduction of nitrogen oxides. *Catal. Sci. and Technol.* 15 (2), 547–562. doi: 10.1039/D4CY01205D

Busca, G., Lietti, L., Ramis, G., and Berti, F. (1998). Chemical and mechanistic aspects of the selective catalytic reduction of NO by ammonia over oxide catalysts: a review. *Appl. Catal. B Environ.* 18 (1–2), 1–36. doi: 10.1016/S0926-3373(98)00040-X

Cardoso, J. S., Silva, V., Rocha, R. C., Hall, M. J., Costa, M., and Eusébio, D. (2021). Ammonia as an energy vector: current and future prospects for low-carbon fuel applications in internal combustion engines. *J. Clean. Prod.* 296, 126562. doi: 10.1016/j.jclepro.2021.126562

Chen, Z., Wang, F., Li, H., Yang, Q., Wang, L., and Li, X. (2012). Low-temperature selective catalytic reduction of NO_x with NH_3 over Fe–Mn mixed-oxide catalysts containing Fe_3 Mn_3 O_8 phase. *Industrial and Eng. Chem. Res.* 51 (1), 202–212. doi: 10.1021/ie201894c

Damma, D., Ettireddy, P., Reddy, B., and Smirniotis, P. (2019). A review of low temperature NH3-SCR for removal of NOx. *Catalysts* 9 (4), 349. doi: 10.3390/catal9040349

Fickel, D. W., and Lobo, R. F. (2010). Copper coordination in Cu-SSZ-13 and Cu-SSZ-16 investigated by variable-temperature XRD. *J. Phys. Chem. C* 114 (3), 1633–1640. doi: 10.1021/jp9105025

Gao, F., Walter, E. D., Karp, E. M., Luo, J., Tonkyn, R. G., Kwak, J. H., et al. (2013). Structure–activity relationships in NH3-SCR over Cu-SSZ-13 as probed by reaction kinetics and EPR studies. *J. Catal.* 300, 20–29. doi: 10.1016/j.jcat.2012.12.020

Glarborg, P. (2022). The NH 3/NO 2/O 2 system: constraining key steps in ammonia ignition and N 2 O formation. *Combust. Flame* 257, 112311. doi: 10.1016/j.combustflame.2022.112311

Gopinathan, R. L., and Mohamed Ibrahim, M. (2025). Ammonia as a sustainable fuel for diesel engines: exploring advanced combustion strategies for green transportation. *J. Energy Inst.* 121, 102159. doi: 10.1016/j.joei.2025.102159

Guan, B., Zhan, R., Lin, H., and Huang, Z. (2014). Review of state of the art technologies of selective catalytic reduction of NOx from diesel engine exhaust. *Appl. Therm. Eng.* 66 (1–2), 395–414. doi: 10.1016/j.applthermaleng.2014.02.021

Guo, Y. (2017). "Experimental and numerical analysis of NOx reduction in marine urea-SCR system', 2017 4th international conference on information, cybernetics and computational social systems (ICCSS). 2017 4th international conference on information, cybernetics and computational social systems (ICCSS),". Dalian: IEEE, 450–455. doi: 10.1109/ICCSS.2017.8091457

IPCC (2021). *Climate Change 2021: The Physical Science Basis. Contribution of Working Group I to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change*. Cambridge University Press. doi: 10.1017/9781009157896

Jung, Y., Pyo, Y., Jang, J., Woo, Y., Ko, A., Kim, G., et al. (2022). Nitrous oxide in diesel aftertreatment systems including DOC, DPF and urea-SCR. *Fuel* 310, 122453. doi: 10.1016/j.fuel.2021.122453

Kobayashi, H., Hayakawa, A., Somarathne, K., and Okafor, E. (2019). Science and technology of ammonia combustion. *Proc. Combust. Inst.* 37 (1), 109–133. doi: 10.1016/j.proci.2018.09.029

Koebel, M., Elsener, M., and Kleemann, M. (2000). Urea-SCR: a promising technique to reduce NOx emissions from automotive diesel engines. *Catal. Today* 59 (3–4), 335–345. doi: 10.1016/S0920-5861(00)00299-6

Kuta, K. K, Nadimi, E., Przybyła, G., Żmudka, Z., and Adamczyk, W. (2022). Ammonia CI engine aftertreatment systems design and flow simulation. *Combust. Engines* 190 (3), 3–10. doi: 10.19206/CE-143158

Kuta, K., Przybyła, G., Kurzydym, D., and Żmudka, Z. (2023). Experimental and numerical investigation of dual-fuel CI ammonia engine emissions and after-treatment with V2O5/SiO2–TiO2 SCR. *Fuel* 334, 126523. doi: 10.1016/j.fuel.2022.126523

Lesmana, H., Zhang, Z., Li, X., Zhu, M., Xu, W., and Zhang, D. (2019). NH3 as a transport fuel in internal combustion engines: a technical review. *J. Energy Resour. Technol.* 141 (7), 070703. doi: 10.1115/1.4042915

Lesmana, H., Zhu, M., Zhang, Z., Gao, J., Wu, J., and Zhang, D. (2021). Experimental and kinetic modelling studies of flammability limits of partially dissociated NH3 and air mixtures. *Proc. Combust. Inst.* 38 (2), 2023–2030. doi: 10.1016/j.proci.2020.06.248

Lhuillier, C., Brequigny, P., Lamoureux, N., Contino, F., and Mounaïm-Rousselle, C. (2020). Experimental investigation on laminar burning velocities of ammonia/hydrogen/air mixtures at elevated temperatures. *Fuel* 263, 116653. doi: 10.1016/j.fuel.2019.116653

Liu, S., Li, H., Liew, C., Gatts, T., Wayne, S., Shade, B., et al. (2011). An experimental investigation of NO2 emission characteristics of a heavy-duty H2-diesel dual fuel engine. *Int. J. Hydrogen Energy* 36 (18), 12015–12024. doi: 10.1016/j.ijhydene.2011.06.058

Liu, F., Yu, Y., and He, H. (2014). Environmentally-benign catalysts for the selective catalytic reduction of NO_x from diesel engines: Structure–Activity relationship and reaction mechanism aspects. *Chem. Commun.* 50 (62), 8445–8463. doi: 10.1039/C4CC01098A

Liu, Z., Luo, J., Pan, Y., Li, J., Li, L., Wei, X., et al. (2023). Multi-objective optimization of the performance and emission characteristics for a dual-fuel engine with hydrogen addition. *Fuel* 332, 126231. doi: 10.1016/j.fuel.2022.126231

Lott, P., and Deutschmann, O. (2023). Heterogeneous chemical reactions—A cornerstone in emission reduction of local pollutants and greenhouse gases. *Proc. Combust. Inst.* 39 (3), 3183–3215. doi: 10.1016/j.proci.2022.06.001

Madia, G., Koebel, M., Elsener, M., and Wokaun, A. (2002). Side reactions in the selective catalytic reduction of NO $_x$ with various NO_2 fractions. *Industrial and Eng. Chem. Res.* 41 (16), 4008–4015. doi: 10.1021/ie020054c

Mørch, C. S., Bjerre, A., Gøttrup, M., Sorenson, S., and Schramm, J. (2011). Ammonia/Hydrogen mixtures in an SI-engine: engine performance and analysis of a proposed fuel system. *Fuel* 90 (2), 854–864. doi: 10.1016/j.fuel.2010.09.042

Nicosia, D., Czekaj, I., and Kröcher, O. (2008). Chemical deactivation of V2O5/WO3–TiO2 SCR catalysts by additives and impurities from fuels, lubrication oils and urea solution. *Appl. Catal. B Environ.* 77 (3–4), 228–236. doi: 10.1016/j.apcatb.2007.07.032

Nova, I., Ciardelli, C., Tronconi, E., Chatterjee, D., and Weibel, M. (2009). Unifying redox kinetics for standard and fast NH_3 -SCR over a V_2 O_5 -WO_3/TiO_2 catalyst. *AIChE J.* 55 (6), 1514–1529. doi: 10.1002/aic.11750

Nova, I., Colombo, M., and Tronconi, E. (2011). Kinetic modeling of dynamic aspects of the standard NH_3 -SCR reaction over V_2 O_5 -WO_3/TiO_2 and Fe-Zeolite commercial catalysts for the aftertreatment of diesel engines exhausts. *Oil and Gas Sci. Technol. – Revue D'IFP Energies Nouvelles* 66 (4), 681–691. doi: 10.2516/ogst/2011132

Ogidiama, O. V. (2014). *Modeling and Optimization of Selective Catalytic Reduction (SCR) Systems for Post-combustion Nox Control*. Abu Dhabi: MSc Thesis. Available online at: https://khazna.ku.ac.ae/en/studentTheses/modeling-and-optimization-of-selective-catalytic-reduction-scr-sy (Accessed May 15, 2026).

Okafor, E. C., Naito, Y., Colson, S., Ichikawa, A., Kudo, T., Hayakawa, A., et al. (2019). Measurement and modelling of the laminar burning velocity of methane-ammonia-air flames at high pressures using a reduced reaction mechanism. *Combust. Flame* 204, 162–175. doi: 10.1016/j.combustflame.2019.03.008

Olsson, L., Sjövall, H., and Blint, R. J. (2008). A kinetic model for ammonia selective catalytic reduction over Cu-ZSM-5. *Appl. Catal. B Environ.* 81 (3–4), 203–217. doi: 10.1016/j.apcatb.2007.12.011

Otomo, J., Koshi, M., Mitsumori, T., Iwasaki, H., and Yamada, K. (2018). Chemical kinetic modeling of ammonia oxidation with improved reaction mechanism for ammonia/air and ammonia/hydrogen/air combustion. *Int. J. Hydrogen Energy* 43 (5), 3004–3014. doi: 10.1016/j.ijhydene.2017.12.066

Paolucci, C., Khurana, I., Parekh, A. A., Li, S., Shih, A. J., Li, H., et al. (2017). Dynamic multinuclear sites formed by mobilized copper ions in NO_x selective catalytic reduction. *Science* 357 (6354), 898–903. doi: 10.1126/science.aan5630

Pedersen, K. A., Lewandowski, M. T., Schulze-Netzer, C., Pasternak, M., and Løvås, T. (2023). Ammonia in dual-fueled internal combustion engines: impact on NO_x, N_2 O, and soot formation. *Energy and Fuels* 37 (22), 17585–17604. doi: 10.1021/acs.energyfuels.3c02549

Ramis, G., Yi, L., and Busca, G. (1996). Ammonia activation over catalysts for the selective catalytic reduction of NOx and the selective catalytic oxidation of NH3. An FT-IR study. *Catal. Today* 28 (4), 373–380. doi: 10.1016/S0920-5861(96)00050-8

Reiter, A. J., and Kong, S.-C. (2011). Combustion and emissions characteristics of compression-ignition engine using dual ammonia-diesel fuel. *Fuel* 90 (1), 87–97. doi: 10.1016/j.fuel.2010.07.055

Schaber, P. M., Colson, J., Higgins, S., Thielen, D., Anspach, B., and Brauer, J. (2004). Thermal decomposition (pyrolysis) of urea in an open reaction vessel. *Thermochim. Acta* 424 (1–2), 131–142. doi: 10.1016/j.tca.2004.05.018

Shi, Z., Peng, Q., E, J., Xie, B., Wei, J., Yin, R., et al. (2023). Mechanism, performance and modification methods for NH3-SCR catalysts: a review. *Fuel* 331, 125885. doi: 10.1016/j.fuel.2022.125885

Shin, Y., Jung, Y., Cho, C. P., Pyo, Y. D., Jang, J., Kim, G., et al. (2020). NOx abatement and N2O formation over urea-SCR systems with zeolite supported Fe and Cu catalysts in a nonroad diesel engine. *Chem. Eng. J.* 381, 122751. doi: 10.1016/j.cej.2019.122751

Song, X., Johnson, J. H., and Naber, J. D. (2015). A review of the literature of selective catalytic reduction catalysts integrated into diesel particulate filters. *Int. J. Engine Res.* 16 (6), 738–749. doi: 10.1177/1468087414545094

Valera-Medina, A., Xiao, H., Owen-Jones, M., David, W., and Bowen, P. (2018). Ammonia for power. *Prog. Energy Combust. Sci.* 69, 63–102. doi: 10.1016/j.pecs.2018.07.001

Voglar, J., Teržan, J., Kroflič, A., Huš, M., and Likozar, B. (2023). Mechanistic modelling of catalytic NOX reduction reactions after hydrogen or ammonia combustion on multiple scales. *Renew. Sustain. Energy Rev.* 186, 113666. doi: 10.1016/j.rser.2023.113666

Wang, Z., Zhu, Y., Zhou, S., and Feng, Y. (2020). Reaction mechanism and chemical kinetics of NH_3 -NO/NO_2 -SCR system with vanadium-based catalyst under marine diesel exhaust conditions. *Proc. Institution Mech. Eng. Part A J. Power Energy* 234 (3), 342–352. doi: 10.1177/0957650919857618

Wu, M., Cova-Bonillo, A., Gabana, P., Brinklow, G., Khedkar, N., Herreros, J., et al. (2024). Addressing the challenge of ammonia slip and nitrous oxide emissions from zero-carbon fuelled engines through catalytic aftertreatment solutions. *Int. J. Hydrogen Energy* 94, 848–861. doi: 10.1016/j.ijhydene.2024.11.173

Yao, D., Hu, X., Wu, F., Li, X., and Li, Y. (2023). Hydrothermal aging mechanism and modeling for SCR catalysts. *ACS Omega* 8 (2), 2421–2434. doi: 10.1021/acsomega.2c06902

Zhang, K., Luo, N., Huang, Z., Zhao, G., Chu, F., Yang, R., et al. (2023). Recent advances in low-temperature NH3-SCR of NOx over Ce-based catalysts: performance optimizations, reaction mechanisms and anti-poisoning countermeasures. *Chem. Eng. J.* 476, 146889. doi: 10.1016/j.cej.2023.146889

Zhao, Q., Yang, Q., Xu, H., Jiao, A., and Pan, D. (2023). Experimental study on pollutant emission characteristics of diesel urea-based selective catalytic reduction system based on corrugated substrate. *Energy* 267, 126475. doi: 10.1016/j.energy.2022.126475

Zhou, J., Guo, R. t., Zhang, X. f., Liu, Y. z., Duan, C. p., Wu, G. l., et al. (2021). Cerium oxide-based catalysts for low-temperature selective catalytic reduction of NO_x with NH_3: a review. *Energy and Fuels* 35 (4), 2981–2998. doi: 10.1021/acs.energyfuels.0c04231

Zhuang, Z., Guan, B., Chen, J., Zheng, C., Zhou, J., Su, T., et al. (2024). Review of nitrous oxide direct catalytic decomposition and selective catalytic reduction catalysts. *Chem. Eng. J.* 486, 150374. doi: 10.1016/j.cej.2024.150374