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# Modeling the efficiency of SCR catalyst in the exhaust system

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***Abstract*— Future automotive application requires safe, clean, and efficient engines as there will be higher mobility on one hand and lesser resources on the other hand. The development of diesel engines has paved the way for improved efficiency, power, and emissions. The main challenge faced by the automotive industry is the reduction of pollution emission. Hence the emission control system needs an improved exhaust after-treatment system to satisfy the stringent emission norms. Selective Catalytic Reduction (SCR) has proven as the best way for the removal of nitrogen oxides (NOX) from the exhaust gas. Proper reduction of Nox depends on various factors like catalyst and arrangements.**

**Keywords—SCR, Chemical kinetics**

## I. Introduction

The automobile industry has not only made life easy and convenient but also susceptible to toxic emissions and the risk of accidents. The urban individuals are suffering most of the fumes of automobile exhaust, because of the incomplete combustion of the fuel, pollutants such as NOx, CO, HC are emitted into the atmosphere. These pollutants cause an associated adverse impact on human health still setting that involves tight emission legislation norms. Studies have shown that people eupneic these pollutants became victims of metabolic processes, biological processes, and skin issues. Once considering the four-stroke engine, the exhaust is the final stage. Diesel is a mixture of hydrocarbons, which produces N2, O2, CO2, and H2O along with NOx, CO, particulate matter and unburnt hydrocarbons after combustion. Out of those waste product emissions, the oxides of nitrogen's square measure thought of because of the most harmful waste product to human health, plants, and environments. Among many technologies from the exhaust gas treatment system SCR (Selective Catalytic Reduction) is considered the most effective one.

SCR is a lively emission management technique utilized in diesel systems to manage the Nox emission from the tailpipe of the exhaust system. SCR performs the selective catalytic reduction of harmful nitrous oxide ($NO_x$) to nitrogen ($N_2$) and water ($H_2O$). The SCR technology injects a liquid reductant through the catalyst into the engine exhaust stream. The reducing agent for the conversion of $NO_x$ is $NH_3$.

The challenge in the exhaust is to find a proper method to reduce the pollutant emission with good efficiency. This paper discusses various modifications in SCR technology and proposes a new methodology that can achieve 100% efficiency compared to others.

## II. LITERATURE SURVEY

Lots of studies square measures conducted for the economical reduction of Nox from the exhaust of the engine. Some studies related to Nox reduction using SCR catalysts are closely observed and reviewed here.

In SCR storing and injection of ammonia has its disadvantages. This can be often because; NH3 should be stored in highly pressurized tanks and is toxic to the beings on earth. Hence a leak within the NH3 tank can affect the environment furthermore as its inhabitants. Wolfgana Held et al.has made two conclusions that the employment of urea is usually considered as safe.It is easy to transport in the vehicle in an aqueous solution, which makes it also easy to dose as required and Copper-exchanged zeolite catalysts can selectively convert nitrogen oxides over a much wider range of fuel-air ratios than Nobel-metal catalysts.[1]

Supported tests conducted, Cu/ZSM-5 (catalyst has been tested in each laboratory and a awfully gasoline-fueled, lean-burn automobile) is mostly believed to be the current "state of the art" for removing NOx from lean engine exhaust. The laboratory tests showed that the HC species was the exhaust component which reduced the NOx. This catalyst produced CO, but the CO had no impact on the NOx reduction. The NOx conversion was inhibited by oxygen at oxygen levels below 4% but was also modestly inhibited by oxygen levels above 4%. The NOx, conversion of those catalysts was less affected by SO2 than were the HC and CO conversions. These catalysts showed very poor thermal durability, losing much of their activity after aging under conditions milder than those typically used for three-way catalysts. The vehicle tests of the fresh Cu/ZSM-5 catalyst showed between 30 and 40% average NOx conversion. [2]

Further studies are done to achieve Nox reduction underneath lean diesel exhaust gas conditions by employing a special coated, zeolite-based monolith catalyst. Abundant attention is paid to the advance of the activated zeolite system and therefore influence of group Ib and VIII elements of the periodic system. Experiments are conducted to find the influence of hydrocarbons, carbon monoxide, sulfur dioxide, and water on the activity of the catalyst. Another aspect discussed is that the influence of the residence time of the exhaust gas components. The thermal stability and also the influence of poisoning elements on the catalyst performance are demonstrated by model gas reactor tests on kitchen appliances and engine aged samples [3]. Under the lean condition, Cu-zeolite is suitable for the decomposition of NO. Copper ion-exchanged ZSM-5, as an example, known to decompose NO into N2 and O2.

Copper ion-exchanged X-zeolite with urea infusion was tested for NOx conversion efficiency by Nag and Gosh Temperature information points were obtained to create peak activation temperatures. Air/fuel ratio have a desired effect on widening of the λ-window; a maximum around 62% NOx conversion efficiency was obtained within the lean-burn range. The consequences of space velocity variations were also observed. To reduce the deactivation of zeolite caused by water, ammonium carbonate and ammonium sulphate was deposited on the copper ion-exchanged X-zeolite and also the corresponding NOx conversion efficiencies measured. [4]

Ammonia slip that's unreacted ammonia prospective pollution hazard, was observed to be more within the case of urea infusion than ammonium salt deposition at higher temperatures. The mechanisms of plasma-enhanced selective catalytic reduction of NOx on a V2O5-WO3/TiO2-catalyst were investigated for temperatures between 100 °C and 200 °C by applying numerous analytical methods. [5].Nowadays Cu-beta zeolite catalysts have been developed for mobile applications. Beta zeolite has better durability and a wider temperature range than other catalysts.

Steady state NOx reduction between 150 -300°C, reactivity comparison to identify the necessary hydrocarbon fields for SCR are studied using with and without plasma operations with the help of sodium Y zeolite catalysts. First study conducted was using propene as hydrocarbon, in which NO oxidized into NO2 completely. Further, Plasma-assisted $NO_x$ conversion over the sodium Y zeolite catalyst with supplemental acetaldehyde injection, primarily through the removal of NO from the feed stream. The comparative studies made a conclusion that the thermal catalytic $NO_x$ conversion with acetaldehyde in a NO-containing feed is much higher than that in a $NO_2$-containing feed [6].

Estimation of NOx reduction done on various axial distributions of metals through a catalyst supported numerical model of diesel NOx selective reduction by HC (by considering the adsorption and desorption of HC.).This was really useful information for a design of HC-SCR systems. Sugiura and Harada developed a replacement method of optimization of diesel selective NOx reduction systems with a supplemental HC to enhance the efficiency of HC-SCR [7].

The emission standards (2007) for both light-duty and heavy-duty diesel vehicles was a challenge. About 90% NOx conversion was required to meet the standards. Lean NOx traps (LNTs) and Selective Catalytic Reduction (SCR) of NOx using aqueous (known as Urea SCR) are the technologies used to achieve proper NOx conversion efficiency at low temperature. No new requirement of infrastructure was an advantage of LNT. Urea SCR had high and durable NOx conversion in a wider temperature range, a lower equivalent fuel penalty, and lower system cost. Urea SCR had the best chance of meeting the NOx emission standards. McGill and Khair done some demonstration programs for both light-and heavy-duty applications [8].

SCR of NOx with urea ((NH2)2CO) as reductant is become a promising method for near future diesel exhaust emission control. To achieve a higher conversion rate from NOx to N2 with less NH3 slip in the tail pipe, careful control of dosage of NH3 or urea was necessary. For this, a conventional SCR NOx catalyst usually needs an extra oxidation catalyst for the destruction of excess NH3.To destroy the excess NH3 ,a unique TiO2 -based SCR NOx catalyst was developed, which can be fit into a space for an NOx only catalyst. Self-consuming action in which excess NH3 is partly converted to NO and this secondarily produced NO reacts with the remaining NH3 and finally is reduced to N2 was a main to reduce excess NH3. Such feature can applied to diesel engine vehicles where load changes are frequently observed. Imada and Kikkawa introduced a preliminary result on another TiO2-based SCR NOx catalyst, without vanadium (V) [9].

The ideal ratio of NH3 to NOx molecules (alpha) is 1:1 based on urea consumption and having NH3 available for reaction of all of the exhaust NOx. SCR efficiency can be less than 100% at low temperatures and at higher temperatures with high exhaust SCR catalyst space velocities. The NOx conversion efficiency is low at low temperatures and this was advantageous to reduce the alpha ratio to values less than 1 to avoid NH3 slip. At higher space velocities and temperatures, the conversion efficiency may be higher with alpha ratios greater than 1. Additional NH3 slip was a concern under these conditions. Girard and Snow made some experiments on the influence of the alpha ratio on NOx conversion efficiency for High and Low-Temperature SCR formulations and concluded that alpha ratio can be less than or greater than 1. At higher temperatures NH3 can oxidize over an SCR catalyst, so overdosing of urea can lead improved NOx conversion efficiency without NH3 slip. At low temperatures, alpha is slightly less than 1 to slightly greater than 1 and conversion efficiency is almost independent of alpha, so that the NH3 slip can be reduced without affecting NOx conversion efficiency [10].

When the urea solution is injected into the exhaust system, it will undergo hydrolysis and decomposition reaction that produces ammonia. Ammonia will react with the exhaust gases to convert NOx into nitrogen, N2, and water, H2O at the catalytic surface. One of the difficult issues was to make sure that the urea solution is available for the SCR system at cold start conditions. At low ambient temperatures, a heating system is required to provide the heat required for melting the frozen urea (At starting stage of the vehicle). There will be some time difference between the vehicle start-up and the availability of urea solution. The time taken by the urea tank heating system to deliver adequate quantities of urea solution depends on the initial temperature, the mass of the frozen urea, heating system design, and dimensions. A transient thermal analysis model is developed in [11] which describing heating process. Test data for the warm-up time at different test conditions also presented.

On the idea of dynamic operation mode of urea SCR systems, improved control strategies are required to reinforce urea dosing control. Zahu and chen introduced a brand new control-oriented model presentation of urea-SCR systems. A controller supported the triple-step non-linear method is meant to track the different ammonia coverage ratio. This system provides a concise design process so that the derivation of the control law is simple. The hardiness of the controller against measurement noises and system uncertainties is analyzed. A transient simulation is conducted to evaluate the effectiveness of the control strategy [12]

Different catalyst investigated for the low-temperature SCR of NOx with ammonia. Among all Cu/TiO2 showed high de-NOx performance in the temperature range of 150-200 °C followed by Mn/TiO2 in the temperature range of 200-250 °C. The Ce/TiO2 catalyst exhibited a broad temperature window with significant de-NOx performance in the temperature range of 250-350 °C. The results of those studies showed that the activity enhancement was correlated with the properties of the support material. All the anatasetitania-supported catalysts demonstrated high de-NOx performance above 150 °C.. Future low emissions standards for light duty diesel and gasoline engine vehicles are forcing automobile and catalyst manufacturers to focus on reducing cold start and low load NOx emissions. These legislations implement very stringent limits on NOx emissions and trigger a renewed attention in NOx mitigation at low temperatures. Light duty diesel and gasoline vehicles will require >95% NOx conversion. This requirement is demanding for the low temperature exhaust applications (mostly operate in the 100-350°C temperature regime- cold start) .Low temperature SCR catalyst systems are considered as good alternative solution to problems associated with the existing catalytic systems during the cold start and low idle conditions. Kotrba and Spinks developed some low temperature catalysts and investigated for catalytic reduction of NOx in the temperature range between 100 and 500 °C [13].

From all these studies made an understanding that temperature, nature of catalyst, space velocity, frequency, NH3 Slip, NOx slip and etc. are considered as a critical factors in NOx conversion efficiency.

When considering a correct way to inject urea, mapping technology was used for the reduction of NOx by measuring the previous output value of NOx. Lean of ammonia causes NOx slip which is undesirable because it won't suit the emission standards. At the same time, injection of excess amount than what the catalyst can hold, causes NH3 slip. Else, NH3 may react with excess O2 to produce NOx again. Thus the management within the quantity of ammonia injection into the exhaust stream plays a big role in deciding the products which will be released into the atmosphere. A new urea dosing system of SCR with flow feedback, a flow sensor and different control methods is proposed [14]. The proposed system embeds all the control elements within the flow rate regulation, which successfully solves the precise control of the urea dosing system with nonlinear dynamics.

When considering the studies, the main aim behind these modifications of catalyst and dosing system was nothing but to enhance the efficiency of the SCR catalyst. That is a proper conversion of NOx to $N_2$.In the SCR system, proper injection of urea is also a factor. A new model an estimated way to find the efficiency of the catalyst based on chemical kinetics which influences the amount of ammonia to be injected is proposed here. The modern approach is to determine the efficiency using kinetics of the reactions in the system.

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A new system model for $NO_x$ reduction with the SCR technology is proposed here. Various factors have to be considered to find the right amount of ammonia to be injected. Efficiency of the catalyst is a main factor among them. The proposed system aims to model the efficiency of the SCR catalyst based on the kinetics of the $NO_x$ reactions.

The desired reaction for modeling is

$$4NO + 4NH_3 + O_2 \rightarrow 4N_2 + 6H_2O \quad (1)$$

Efficiency here is defined as below:

$$\text{Efficiency}(\eta) = 1 - \frac{[NO]_{downstream}}{[NO]_{upstream}} \quad (2)$$

Hence the concentration of $NO_x$ before and after passing through the catalyst can be modelled as Hence the concentration of $NO_x$ before and after passing through the catalyst can be modelled as:

$$\frac{[NO]_{downstream}}{[NO]_{upstream}} = e^{-k*t} \quad (3)$$

Where k is the rate of the reaction and t is the dwell time of $NO_x$ in catalyst. Therefore the overall efficiency of the catalyst is modelled as:

$$\text{Efficiency } (\eta) = 1 - e^{-k*t} \quad (4)$$

## III. CONCLUSION

To meet the stringent emission norms for $NO_x$ into the atmosphere, the introduction of the SCR system in the exhaust system of automobiles is essential. The control algorithm to inject the right amount of ammonia should be designed expertly. The efficiency of the catalyst is one such factor that decides the amount of $NH_3$ to be injected. A model-based method to find the efficiency of the catalyst using kinetics is introduced here. The maximum efficiency that can be achieved with the model is 1 and the minimum is 0.

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