

# Performance Analysis of the Control of NOx Emissions from the Hydrogen Engine

Muthuraman Subbiah<sup>1\*</sup>, Sivaraj Murugan<sup>2</sup>, Kumar Ayyappan<sup>3</sup>

<sup>1</sup>Department of Engineering, University of Technology and Applied Sciences, Muscat, Oman

<sup>2</sup>Department of Mechanical Engineering, Rohini College of Engineering and Technology, TN- India

<sup>3</sup>Department of Applied Sciences, Amrita College of Engineering and Technology, TN- India

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\*Corresponding author: Muthuraman Subbiah

Department of Engineering, University of Technology and Applied Sciences, Muscat, Oman

## Abstract

Hydrogen serves as an optimal fuel for engines. Pure hydrogen engines do not generate carbon monoxide and hydrocarbon emissions; instead, they encounter significant nitrogen oxide emissions. Inner-engine control and outer-engine control are two methods to reduce NOx emissions. Outer-engine control primarily mitigates NOx emissions by selective catalytic reduction (SCR), a process that has been extensively researched. Nevertheless, there is a paucity of research about NOx emission regulation in pure hydrogen engines via internal engine management. This work utilised the closed homogeneous reactor (CHR) in Chemkin Pro to model the primary NOx emission control within pure hydrogen engines. The findings indicate that single exhaust gas recirculation (EGR) reduces NOx emissions by 45.3% at an EGR ratio of 20%, suggesting that the reduction in NOx emissions is not substantial. Nonetheless, EGR combined with lean burn reduces NOx emissions by 96.31% at a  $\lambda$  of 1.4 and an EGR ratio of 20%, resulting in ultra-low NOx emissions from pure hydrogen engines. In comparison to single EGR and EGR combined with lean-burn, SNCR is more effective for NOx emission control. An NH<sub>3</sub> ratio of merely 10% can reduce NOx emissions by 96.32% in pure hydrogen engines, whilst a 15% NH<sub>3</sub> ratio can attain zero NOx emissions in pure hydrogen engines without necessitating a high  $\lambda$  value or EGR ratio. It is essential to precisely regulate the NH<sub>3</sub> ratio in the cylinder; otherwise, residual NH<sub>3</sub> may be generated, leading to environmental pollution.

**Keywords:** NOx Emissions, Lean Burn, Hydrogen Engine, Selective Non-Catalytic Reduction (SNCR), Exhaust Gas Recirculation (EGR).

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## 1. INTRODUCTION

The extensive use of fossil fuels has resulted in significant pollution issues. Pursuing clean and efficient renewable energy may address pollution issues and mitigate the energy crisis. Hydrogen is a sustainable fuel whose sole combustion byproduct is water, posing no environmental harm [1, 2]. Utilising pure hydrogen in engines can nearly eliminate CO, CO<sup>2</sup>, and unburned hydrocarbon pollutants, while producing greater power than pure petrol. However, NOx emissions represent the primary drawback of pure hydrogen engines. The primary technical methods to mitigate NOx emissions include exhaust gas recirculation (EGR) technology, EGR combined with lean burn technology, selective non-catalytic reduction (SNCR) technology, and selective catalytic reduction (SCR) technology [3, 4]. The outside engine control primarily mitigates NOx emissions via

SCR, which has been extensively researched. The primary methods for controlling NOx emissions within engines currently include EGR technology, EGR combined with lean-burn technology, and SNCR technology. Nevertheless, there is a paucity of research about NOx emission regulation in pure hydrogen engines via internal engine management [5-8]. This paper simulated and compared three primary methods for controlling NOx emissions in pure hydrogen engines, offering a theoretical foundation for selecting technical approaches to mitigate NOx emissions in these engines [9, 10].

## 2. Setup and Procedure

The simulation program employed in this analysis was Chemkin Pro, and the model utilised was a closed homogeneous reactor (CHR). The H<sub>2</sub> combustion

mechanism employed in this simulation was the comprehensive mechanism of hydrogen combustion, the NO<sub>x</sub> generation mechanism utilised the enhanced version of the Zeldovich mechanism, and the NO<sub>x</sub> desorption mechanism was supplied by Golovitchev [11-15]. All chemical reaction pathways in the simulation were validated through comprehensive experiments, and the experimental results corresponded precisely with the simulation. This simulation evaluated three internal

engine NO<sub>x</sub> emission reduction technologies: EGR, lean-burn combined with EGR, and SNCR. In this experiment, five  $\lambda$  values (1.1, 1.2, 1.3, 1.4), five EGR ratios (0%, 5%, 10%, 15%, 20%), and five NH<sub>3</sub> ratios (0%, 5%, 10%, 15%, 20%) were established. The EGR ratio is specified in Equation (1), while the NH<sub>3</sub> ratio is delineated in Equation (2). Table 1 presents the initial conditions for the closed homogeneous reactor.  $V_x$  denoted the volume of  $x$  in the subsequent equations.

**Table 1: Closed homogeneous reactor parameter and values**

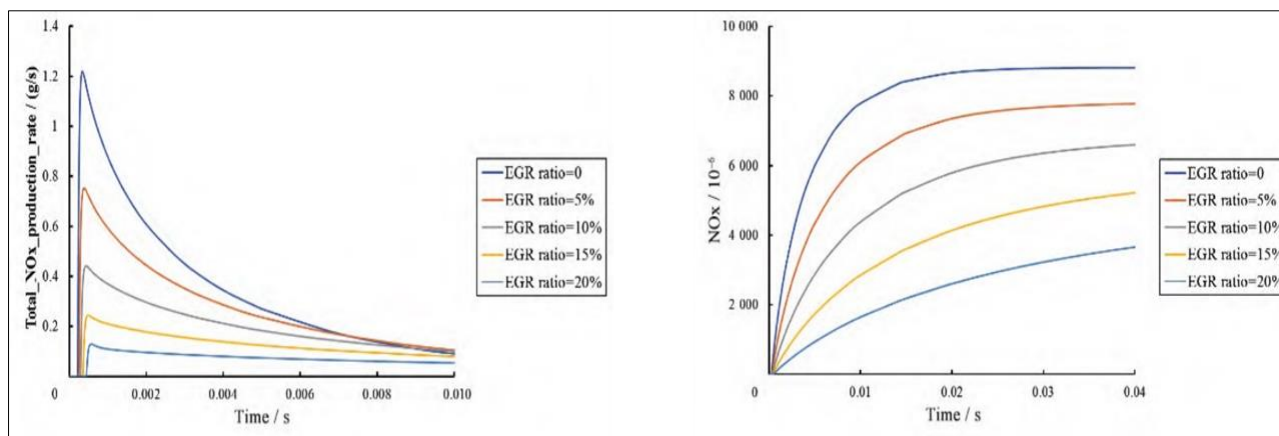
S No	Parameters	Values
1	Simulation time/s	0.04
2	Initial temperature/K	1000
3	Initial pressure/MPa	0.1
4	Mixture (vol)	$\phi(\text{H}_2) = 100\%$
5	Oxidizer mixture (vol)	$\phi(\text{O}_2) = 21\%$ , $\phi(\text{N}_2) = 79\%$
6	Added species	$\text{H}_2\text{O}$ ; $\text{N}_2$ ; $\text{NH}_3$
7	Excess air ratio	1, 1.1, 1.2, 1.3, 1.4

### 3. RESULTS AND DISCUSSION

#### 3.1 Cause of EGR on NO<sub>x</sub> Emission

Figure 1 illustrates the impact of Exhaust Gas Recirculation (EGR) on the overall nitrogen oxides (NO<sub>x</sub>) production rate and NO<sub>x</sub> emissions. Figure 1 illustrates that an increase in the EGR ratio results in a reduction of both the peak total NO<sub>x</sub> generation rate and the overall NO<sub>x</sub> emissions. As the EGR ratio escalates from 0% to 20%, the maximum total NO<sub>x</sub> production rate diminishes by 38.52%, 63.93%, 80.33%, and

89.34%, respectively. The overall NO<sub>x</sub> emissions diminish by 11.42%, 22.82%, 34.18%, and 45.30%. The conditions for NO<sub>x</sub> generation include elevated temperatures, oxygen enrichment, and prolonged high temperatures. The augmentation of the EGR ratio diminishes the cylinder temperature while concurrently diluting the concentrations of N<sub>2</sub> and O<sub>2</sub>, so decreasing the NO<sub>x</sub> production rate. Consequently, the implementation of EGR technology can significantly diminish NO<sub>x</sub> emissions produced during hydrogen combustion.

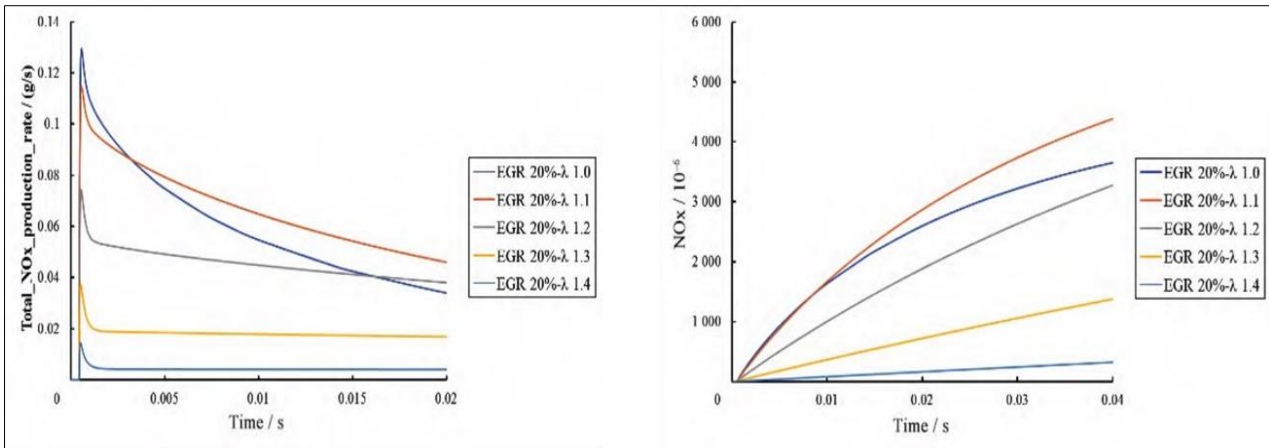


**Fig. 1: EGR on total NO<sub>x</sub> production rate and NO<sub>x</sub> emission**

#### 3.2 Impact of EGR plus Lean-Burn on NO<sub>x</sub> Emission

The EGR ratio was maintained at 20%, but the surplus air ratio was elevated from 1 to 1.4 to examine the impact of EGR combined with lean-burn on NO<sub>x</sub> emissions. Figure 2 illustrates the impact of Exhaust Gas Recirculation (EGR) combined with lean-burn on the overall nitrogen oxides (NO<sub>x</sub>) production rate and emissions. The maximum total NO<sub>x</sub> production rate consistently declined with increasing  $\lambda$ , while NO<sub>x</sub> emissions initially rose and subsequently fell as  $\lambda$

increased. At a  $\lambda$  of 1.1, the NO<sub>x</sub> emissions are at their peak. While lean-burn may reduce combustion temperature, an increased  $\lambda$  results in elevated O<sub>2</sub> levels, fostering conditions that enhance oxygen enrichment, hence promoting NO<sub>x</sub> formation. The elevation of oxygen indicates that a combination of a 20% EGR ratio and a  $\lambda$  of less than 1.3 is ineffective in diminishing NO<sub>x</sub> emissions. NO<sub>x</sub> emissions can be diminished by 96.31% when  $\lambda$  is 1.4 and the EGR ratio is 20%.

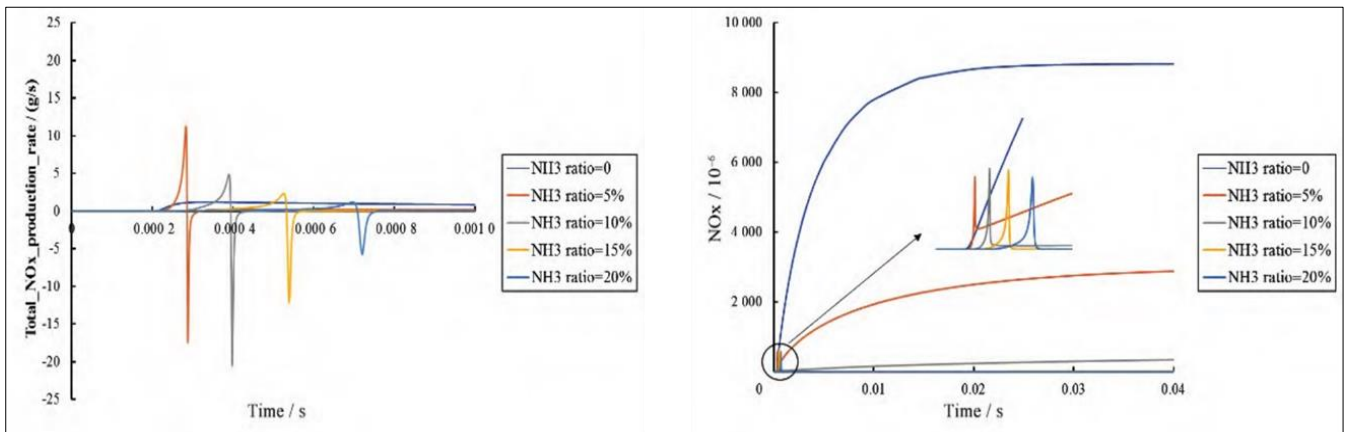


**Fig. 2: EGR plus lean-burn on total NOx production rate and NOx emission**

### 3. 3 Influence of NH<sub>3</sub> on NOx Emission

Figure 3 illustrates the impact of NH<sub>3</sub> on the overall NOx generation rate and NOx emissions. The entire NOx production rate, including positive and negative peak values, consistently declines as the NH<sub>3</sub> ratio increases, while NOx emissions diminish with rising NH<sub>3</sub> ratios.

A higher NH<sub>3</sub> ratio would result in a delayed peak value of the total NOx generation rate. At an NH<sub>3</sub> ratio of 10%, NOx emissions reduce by 96.32% compared to the absence of NH<sub>3</sub> addition, and at an NH<sub>3</sub> ratio of 15%, pure hydrogen engines can attain zero NOx emissions. Nonetheless, a high NH<sub>3</sub> ratio is inadvisable, as excessive residual NH<sub>3</sub> may spill over, resulting non-significant environmental damage.



**Fig. 3: NH<sub>3</sub> on total NOx production rate and NOx emission**

## 4. CONCLUSIONS

This study employed the CHR module in CHEMKIN Pro to simulate the three primary methods of NOx emission control in pure hydrogen engines, offering theoretical assistance for the selection of NOx purification strategies in such engines. The primary findings are as follows:

EGR lowers the NOx emissions produced during hydrogen combustion. The NOx emissions decrease by just 45.3% when the EGR ratio is set at 20%. Consequently, to attain ultra-low NOx emissions with pure hydrogen engines through the implementation of EGR technology, a higher EGR ratio or EGR combined with external purification must be utilised.

In comparison to single EGR, the combination of EGR and lean burn demonstrates superior efficiency

in diminishing NOx emissions when utilising pure hydrogen engines. Pure hydrogen engines require a substantial EGR ratio and lambda value. NOx emissions can be diminished by 96.31% when  $\lambda$  is 1.4 and the EGR ratio is 20%, resulting in ultra-low NOx emissions from pure hydrogen engines. To regulate NOx emissions utilising a pure hydrogen engine alongside EGR and lean-burn technology, it is imperative to enhance engine condition monitoring to prevent misfires resulting from the elevated EGR ratio and  $\lambda$  value.

In comparison to EGR and EGR combined with lean burn, SNCR demonstrates superior control of NOx emissions within the engine, necessitating merely a 10% NH<sub>3</sub> ratio to attain ultra-low NOx emissions in pure hydrogen engines. A 15% NH<sub>3</sub> ratio can enable pure hydrogen engines to attain 0% NOx emissions.

SNCR circumvents the necessity for pure hydrogen engines to function under elevated  $\lambda$  and EGR ratios to mitigate NO<sub>x</sub> emissions, hence preventing power loss and enhancing combustion stability. In managing NO<sub>x</sub> emissions from pure hydrogen engines, SNCR should be the primary technological method employed, and zero emissions can be attained with appropriate regulation of NH<sub>3</sub> levels.

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