Kinetic analysis of the role of selective NO_x recirculation in reducing NO_x emissions from a hydrogen engine

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Highlights

- NO_x injection results in a decrease in further NO_x formation for high equivalence ratios
- Thermodynamic limitations can be used to explain the trends for various amounts of fuel
- Net reduction in NO_x can be obtained even without an interaction between fuel and NO_x
- Operating conditions favoring the net reduction of NO_x identified

1. Introduction

Selective NO_x recirculation (SNR) technique can be used to reduce NO_x emissions from an internal combustion engine. The process consists of selectively adsorbing NO_x from the exhaust using a NO_x adsorber catalyst, followed by desorbing and transporting it to the intake manifold of the engine. Up to 90% reduction in thermal NO_x has been reported by using this technique [1]. Most of the studies explain the reduction in NO_x to the interaction between fuel and NO_x, wherein the fuel acts as a reductant.

In this work, a model based on fundamental conservation equations is used to study the effect of NO injected into a spark ignited H_2 engine on its further formation. Kinetic analysis of the NO_x reduction is performed for various amounts of NO injected into the engine and the operating conditions for achieving high NO_x reduction are deduced. In contrast to the earlier studies on selective NO_x recirculation, it is highlighted that a reduction in NO_x can be achieved even if the reactions between the fuel and NO_x do not take place.

2. Methods

The engine cylinder was assumed to be a well-mixed reactor with a variable volume. Global kinetics were used to describe hydrogen combustion and NO_x formation, which were coupled to the species balance and energy balance equations [2]. The resulting equations were solved simultaneously using MATLAB® to obtain the variation of in-cylinder temperature, pressure and the concentration of various species with time. Simulations were also performed with detailed combustion and decomposition kinetics. The elementary reactions specific to the combustion of hydrogen were extracted from the GRI 3.0 reaction mechanism [3].

In the computational experiments, various amounts of NO were fed into the cylinder during the intake stroke with the inlet concentrations in the range of 0-14000 ppm. The simulations were performed for various fuel-air equivalence ratios (φ) and its effect on the exhaust NO concentration was analyzed. The 'net' NO generated during the cycle was calculated as the difference in the moles of NO in the exhaust during the exhaust stroke and the moles of NO injected during the intake stroke. The NO conversion efficiency was calculated as $\eta=1-(N_{wi}-N_{ow})/N_{feed}$. N_{wi} and N_{wo} respectively represent the moles of NO in the exhaust per cycle with and without the injection of NO, whereas, N_{feed} represents the moles of NO injected in one cycle.

3. Results and discussion

Using the detailed kinetics based on the GRI 3.0 mechanism, the variation of NO conversion efficiency with φ was obtained for various NO concentrations in the inlet air-fuel mixture and the results are shown in Fig. 1. In agreement with the experimental trends reported in the literature for other fuels, the model predicts that high conversion efficiencies are attained for high equivalence ratios. It is also observed that for a fixed value of φ, the conversion efficiency increases with an increase in the fraction of NO during the intake stroke, even though the difference is not very significant. Additionally, the difference between the conversion efficiency becomes lesser with an increase in φ. It was also found that the net amount of NO formed decreased with an increase in φ and the concentration of NO in the intake mixture. Hence, for high values of φ, the selective recirculation of NO_x is expected to result in lower net emissions of NO_x.

To explain the results shown in Fig. 1, the model based on global kinetics was solved to obtain the temporal variation of the in-cylinder NO concentration and the results for φ=0.65 are shown in Fig. 2. The drop in NO concentration during the power stroke is due to the decrease in the in-cylinder temperature, which shifts the equilibrium towards low concentrations of NO. With a further decrease in the temperature, the decomposition of NO is limited by kinetics and hence cannot proceed further. Since the NO concentration approaches equilibrium for high values of φ, the post-ignition NO concentration profiles are not affected to a significant extent by the amount of NO present in the cylinder prior to ignition. This amounts to a reduction in the 'net' moles of NO generated with an increase in the amount of NO injected. However, for low values of φ, the temperatures are lower, due to which the further formation of NO is not limited by equilibrium and hence the injection of NO does not affect its further formation. Most of the studies on SNR explain the conversion of NO_x due to its reaction with the fuel. However, we show that the difference in the approach to equilibrium for various operating conditions can be used to predict the reported experimental trends and that the net NO reduction can be obtained even in the absence of any reactions between the fuel and NO.

The complete manuscript would contain the results on the transient behavior of the complete SNR system, including the engine, adsorber and exhaust gas conditioning before recycling into the intake.

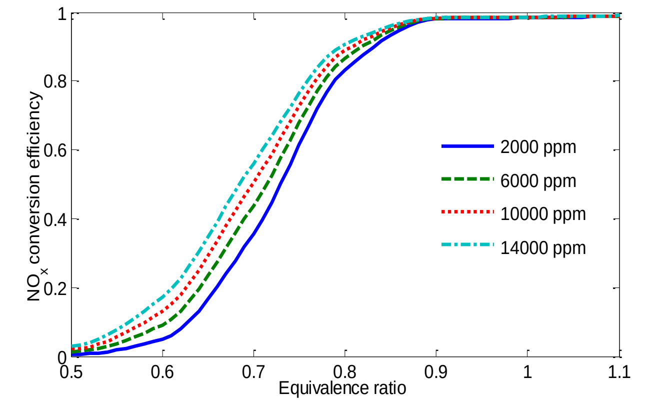

Figure 1. Variation of NO conversion efficiency for various NO fractions in the intake mixture

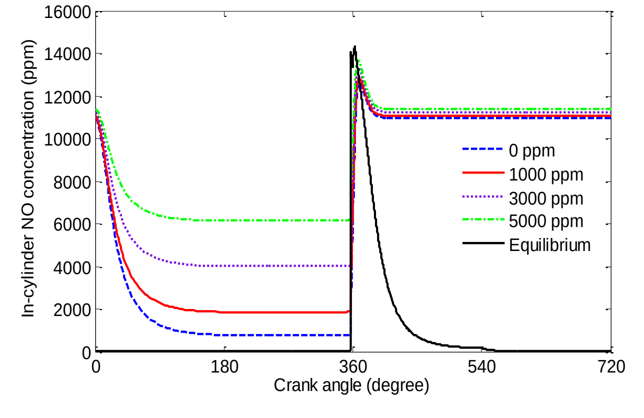

Figure 2. Variation of NO concentration with crank angle for various NO fractions in the intake mixture (φ=0.65)

4. Conclusions

Simulations were performed to study the effect of NO injected into a H_2 engine on its further formation. The use of both global kinetics and detailed kinetics showed that NO reduction is effective for high equivalence ratios and the net reduction in NO is high for high intake concentrations of NO. For operating conditions resulting in high in-cylinder temperatures, the NO formation reaction approaches equilibrium. Hence, the selective adsorption of NO followed by its recirculation into the engine can be used to limit the amount of additional NO produced during the power stroke. Also, a reduction in the net amount of NO generated is predicted even when the reactions between NO and H_2 do not take place. The underlying concept of limiting the NO_x emissions because of thermodynamic limitations should be applicable for any other fuel as well.

References

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Keywords
Selective NO_x recirculation; NO_x injection; NO_x decomposition kinetics; H_2 engine