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Investigating the effect of temperature on NO_x sensor cross sensitivity to ammonia using a physics based model

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1. Abstract

The high level of NO_x emission is one of the most challenging problems of Diesel combustion. Measuring the actual NO_x concentration in the exhaust gas is an important challenge for urea injection control of SCR systems since cross sensitivity of in-use NO_x sensors to ammonia (NH_3), makes it difficult to achieve maximum NO_x conversion in SCR closed-loop control. The effect on the NO_x sensor of temperature and its cross sensitivity to NH_3 is investigated by modeling NH_3 oxidation in the NO_x sensor. The O_2 concentration is then predicted inside the second chamber of the NO_x sensor. The model considers the effect of temperature on NH_3 oxidation products based on three global reactions. N_2O, NO and NO_2 are considered as the main products of NH_3 oxidation inside the sensor. The effect of different NH_3 concentration values on the variation of cross sensitivity factor and O_2 concentration inside the second chamber of the sensor is also studied. The cross sensitivity factor is then determined in terms of NH_3 oxidation products inside the sensor. This model gives insight into physics based analyses of NO_x sensor cross sensitivity to NH_3 as a function of temperature and NH_3 concentration.

2. Introduction

The combustion process of Diesel engines is by a diffusion flame [1]. This increases the NO_x and particulate matter emissions of Diesel engines because of the non homogeneous air-fuel mixture and high temperature inside the combustion chamber [2, 3]. In order to solve this problem, different methods have been developed including Exhaust Gas Recirculation (EGR) [4] and Low Temperature Combustion (LTC) [5]. Among different Diesel NO_x reduction methods, urea-based Selective Catalytic Reduction (SCR) is a promising technique to satisfy future emission standard regulations [6–8].

Developing in-use sensors helps to continuously monitor emissions and to get real-time feedback for combustion control is one method to reduce the engine-out emissions produced during the combustion process. In addition, measuring the actual NO_x concentration is essential for urea injection control of SCR systems because of the cross sensitivity of NO_x sensors to NH_3 . This cross sensitivity makes it difficult to achieve the maximum NO_x conversion in SCR closed-loop control [9–11].

Cross-sensitivity is taken as a constant in [12, 13], a function of time in [14] and the ratio of $\frac{NH_3 concentration}{NO_x concentration}$ in [15]. A dynamic NO_x sensor model is developed in [16] to remove NH_3 cross sensitivity from production NO_x sensors downstream of SCR. The model is validated for large amounts of NH_3 slip during different engine transients and coupled to a nonlinear control oriented SCR model to predict the NH_3 concentration downstream of the SCR and estimate the actual NO_x concentration. Although the cross-sensitivity of NO_x sensors to NH_3 are being actively investigated, improved physics based models are needed to study NH_3 oxidation inside the first chamber of the sensor in more details [17, 18].

The model used in this work is a modified version of the model developed in [18]. The effect of different NH_3

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concentrations on the concentration of each effective species inside the sensor is examined at different sensor temperatures. It is shown that NH_3 concentration has an insignificant effect on the sensor cross sensitivity in steady state condition while temperature directly changes the cross sensitivity by changing the concentration of each species inside the sensor chamber.

3. NO_x sensor model

A schematic view of the NO_x sensor is shown in Figure 1. A zirconia based oxygen pump removes the oxygen molecules (O_2) and converts all NO_x to NO. This process takes place in the first chamber and then NO breaks down into N_2 and O_2 in the second chamber. Finally, the NO_x concentration is calculated based on the O_2 concentration measurement in the second chamber. With the presence of NH_3 in the exhaust gas, NO, NO_2 and N_2O are also produced in the first chamber which directly affects the pumped oxygen from the second chamber and the sensor output.

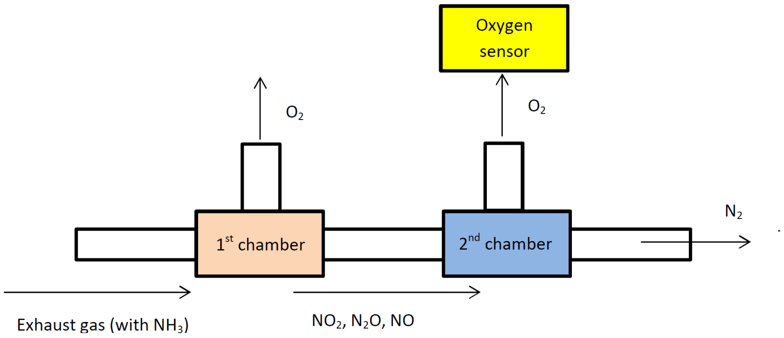

Figure 1: NO_x sensor schematic with the presence of NH_3

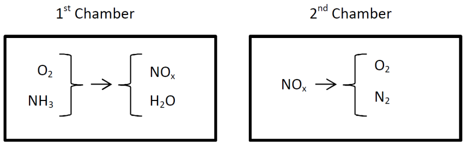

Figure 2: Model Schematic

A linear form of a NO_x sensor model is [19]:

$$C_{NO_x} = C_{NO_{x,sen}} - c_{CS}C_{NH_3} \tag{1}$$

where $C_{NO_{x,sen}}$, c_{CS}, C_{NO_x} and C_{NH_3} are the sensor output signal, the cross sensitivity factor, the actual NO_x and NH_3 concentrations respectively.

The effect of temperature and NH_3 concentration on cross sensitivity of a NO_x sensor to NH_3 is studied by modeling NH_3 oxidation in the first chamber. The oxygen pump is modeled as a constant volume reactor which is open to the transfer of mass. The chamber temperature is assumed to be constant at each operating condition since steady state conditions are assumed and the system is assumed to reach equilibrium. It is assumed that all NO_x is decomposed into N_2 and O_2. Which means O_2 concentration inside the second chamber is directly affected by the temperature of the first chamber. A schematic view of the model is shown in Figure 2.

A simplified physics based model that was previously developed in [18] which solves for energy conservation in which global reaction mechanism for NH_3 oxidation considering 3 reactions and 6 species are used in the first chamber [17,20] is:

$$2NH_3 + 2O_2 \rightarrow N_2O + 3H_2O \tag{2a}$$
$$2NH_3 + 2.5O_2 \rightarrow 2NO + 3H_2O \tag{2b}$$
$$2NH_3 + 3.5O_2 \rightarrow 2NO_2 + 3H_2O \tag{2c}$$

where the equilibrium constants are function of temperature and are defined based on the values reported in [20] and JANAF thermodynamic tables [21].

4. Results and Discussion

To investigate the effect of the temperature in the first chamber (see Figure 1) on cross sensitivity, the temperature is varied between 520 K and 600 K. This range was selected to cover the full effective range of temperature on cross sensitivity that was experimentally studied in [17].

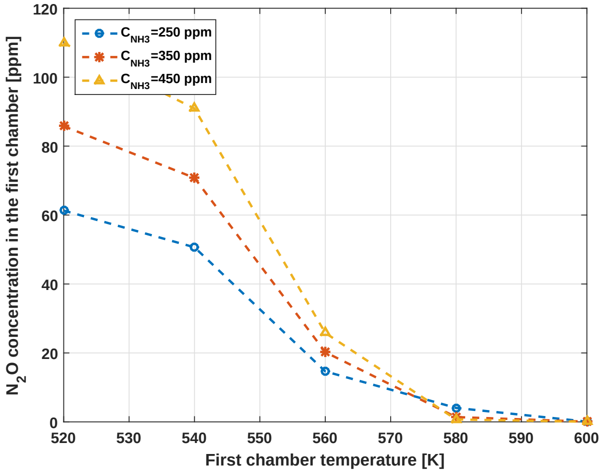

Figure 3: N_2O concentration in the first chamber

The concentrations of N_2O and NO_2 are affected by temperature. As the chamber temperature increases, N_2O concentration decreases while NO_2 concentration increases. At low temperature (around 520 K), Eqn. (2a) is the dominant reaction which means NH_3 is mainly converted to N_2O as shown in Figure 3. However, at high temperature (around 600 K), Eqn. (2c) is the dominant reaction and NH_3 is mainly converted to NO_2 as shown in Figure 4. This results are consistent with [17,20]. Therefore, NH_3 concentration does not affect N_2O concentration at high temperature and NO_2 concentration at low temperature.

It is assumed that the NO_x produced in the first chamber is converted to N_2 and O_2 in the second chamber [17]. The concentrations of O_2, N_2O and NO_2 increase with increasing NH_3 concentration in the exhaust system, as shown in Figure 5, due to NH_3 oxidation in the first chamber. Higher levels of NH_3 in the first chamber results in formation of more N_2O and NO_2 and this increases the O_2 concentration in the second chamber.

For the temperatures higher than 580 K, the O_2 concentration is less sensitive to temperature which is due to the high rate of conversion of NH_3 to N_2O that finally leads to the highest value of cross sensitivity factor which is shown in Figure 6.

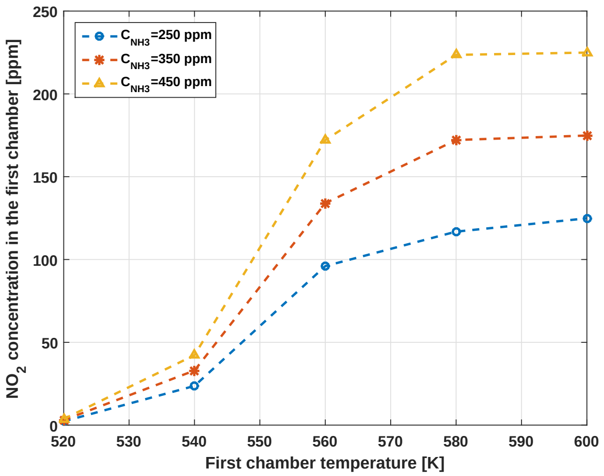

Figure 4: NO_2 concentration in the first chamber

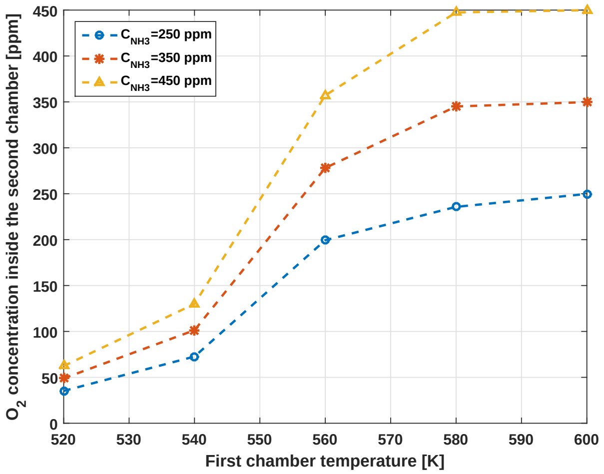

Figure 5: O_2 concentration from NO_x decomposition in chamber 2

Among all of the NH_3 oxidation products, the concentration of N_2O and NO_2 are more important as they are the dominant products at this range of temperature [17]. They directly affect O_2 concentration in the second chamber which is proportional to the sensor output [22] and that is why a NO_x sensor is cross sensitive to NH_3 .

The cross sensitivity factor calculated based on a physics based model is [18]:

$$c_{CS} = c_3 \times (C_{NO} + c_1 \times C_{N2O} + c_2 \times C_{NO2}) \tag{3}$$

where C_{NO}, C_{N_2O} and C_{NO_2} are the NO, N_2O and NO_2 concentrations due to NH_3 oxidation in the first chamber, c_1=0.5, c_2=2 and c_3=$\frac{1}{C_{NH_3}}$.

Despite varying NH_3 concentration, the NO_x sensor cross sensitivity factor is mainly affected by temperature and it remains almost constant as NH_3 concentration changes as shown in Figure 6. This happens since the effect of NH_3 concentration on N_2O concentration and NO_2 concentration is canceled by factor c_3 in Eqn. (3). The cross sensitivity factor varies from 0.25 to 2 as temperature changes from 520 K to 600 K. These results are consistent with the literature [17]. This observation only applies to steady state since NH_3 concentration affects the cross sensitivity factor in transient [16].

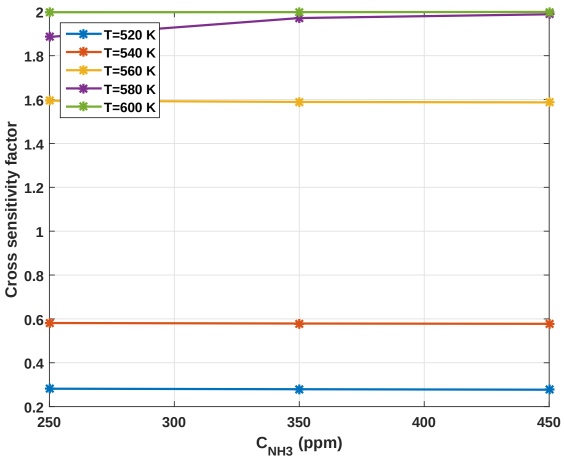

Figure 6: NO_x sensor cross sensitivity factor vs NH_3 concentration

5. Conclusions

The effect of sensor temperature and NH_3 concentration on NO_x sensor cross sensitivity to NH_3 is investigated by modeling NH_3 oxidation inside the sensor. The O_2 concentration is then predicted inside the second chamber as well as N_2O and NO_2 concentrations.

The main conclusions are as following:

- The concentrations of N_2O and NO_2 in the first chamber, increase with increased NH_3 concentration in the exhaust system and this increases the O_2 concentration in the second chamber causing an increase in the sensor output.
- O_2 concentration in the second chamber is increased by increasing temperature as more NH_3 is converted to NO_2 than N_2O.
- Although O_2 concentration in the second chamber is increased with increasing NH_3 concentration, the cross sensitivity factor is a strong function of temperature and a weak function of NH_3 concentration which matches experimental results in the literature.

This analysis gives a physics based insight into modeling the cross sensitivity of a NO_x sensor to NH_3 and the factors that affect it in steady state. Future work will focus the analysis of transient behavior.

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