A New Approach for NOx Soft Sensors for the Aftertreatment of Diesel Engines

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Abstract. To maintain the NOₓ concentration at an appropriate level, traditionally an air-path control that regulates the intake and exhaust system of diesel engines aims to control the mass air flow and the manifold absolute pressure, which influence the production of NOₓ. To improve the control accuracy, a more recent approach takes the NOₓ concentration directly as a controlled output variable, but the sensors monitoring the NOₓ concentration are slow to respond. Consequently, a direct sensor is inappropriate as a feedback controller. Instead a mechanism called a soft sensor, which computes the NOₓ concentration from state quantities of diesel engines, is used. Because the prediction accuracy from the sensor model greatly affects the control performance, it is important to improve the model accuracy. However, deviations in the steady state indicate an insufficient model accuracy. This study proposes a method to construct an adaptive NOₓ soft sensor that corrects the parameters of the sensor model sequentially using the simultaneous perturbation stochastic approximation while comparing the values computed by the software to actual measurements as well as examines the effectiveness of the proposed method experimentally.

1. Introduction

Toward preventing global warming, commercial and passenger vehicles have widely employed diesel engines, which are more thermally efficient and less CO₂-emitting than other internal combustion engines. Because diesel engines using a compression-ignition have a high compression ratio and a large excess air ratio, they are considered to have a higher thermal efficiency. However, they have a serious drawback; due to lean burning, they tend to produce more NOₓ because their combustion chambers are under high-temperature and high-pressure conditions.

A common measure used to reduce the NOₓ emission is an exhaust gas recirculation (EGR) system, which recirculates part of exhaust gas back to the intake manifold. The system is designed to reduce the production of NOₓ by lowering both the temperature of the combustion gas in the chamber and the amount of O₂ in the intake air. This can be accomplished by increasing the gases with a high specific heat capacity, such as CO₂ and H₂O, in the intake air. The flow rate of the recirculated exhaust gas (EGR gas) determines the amount of NOₓ produced. An excess flow may produce diesel particulate...
matter (DPM) or cause a fire accident; therefore, the flow rate of the EGR gas must be controlled appropriately with EGR valves.

A common, conventional method to control the EGR gas flow rate employs a feedback control, where the observed mass air flow (MAF) is taken as the controlled output variable. MAF is kept approximately equal to the predetermined desired air flow rate. However, this system lacks robustness as different boost pressures yield different volumes of NOX emissions even if the system maintains the same MAF rate. Hence, control systems that consider both the intake O2 concentration [1] and NOX concentration [2, 3] as controlled variables have been studied in recent years.

Sensors that monitor these controlled variables usually have slow responses and are inappropriate as feedback controllers. Instead, a mechanism called a soft sensor, which computes the NOX concentration from state quantities of engines, is often adopted. In a soft sensor, the prediction accuracy of the sensor model greatly affects the controllability of the system. Hence, it is important to improve the accuracy of the model, which is insufficient as demonstrated by the deviations in the steady state. Herein a NOX sensor device that measures the actual NOX concentration is a called a "NOX hard sensor", while a sensor that calculates the NOX concentration from other factors is called a "NOX soft sensor".

This study describes a method to construct an adaptive NOX soft sensor that compares the values computed by the NOX soft sensor obtained from an empirical perspective to the output of the NOX hard sensor and corrects the parameters of the sensor model sequentially using the simultaneous perturbation stochastic approximation (SPSA) of the stochastic approximation method. Then actual data obtained from engine bench tests are used to examine the effectiveness of the proposed method.

2. Diesel engine system

2.1. Overview of the diesel engines

Figure 1 shows the overview of the diesel engine system where blue and red indicate the air intake and exhaust systems, respectively.

![Figure 1. Overview of diesel engines.](image-url)
DPM is trapped and accumulated by a diesel particulate filter (DPF) and can be burned off when the accumulation reaches a certain level. NOx is decomposed into water and nitrogen by selective catalytic reduction (SCR) at the appropriate temperature to accelerate the chemical reaction. In SCR, urea is injected and is subsequently hydrolyzed into ammonia and carbon dioxide. The ammonia then renders NOx harmless by reducing it to water and nitrogen via the following chemical reactions

\[
\begin{align*}
(NH_2)_2CO + H_2O & \rightarrow 2NH_3 + CO_2 \\
NO + NO_2 + 2NH_3 & \rightarrow 2N_2 + 3H_2O
\end{align*}
\]

(1)

Reducing the amount of the NOx lead to reduce the urea and cut down the cost of the urea, however, the fuel consumption is deteriorated. Hence, the NOx concentration must be controlled appropriately.

2.2. Direct NOx control

The NOx concentration largely depends on the oxygen concentration, which chiefly drives the rate of combustion. Therefore, conventional methods usually employ the MAF of the fresh intake air, which determines the oxygen concentration, and the manifold absolute pressure (MAP), which is the internal pressure of the intake manifold, as controlled variables. However, the relationship among state quantities in diesel engines is complex. Controlling the amount of NOx indirectly via MAF/MAP leaves many uncertainties. Empirically, the oxygen concentration is closely related to the production of NOx. Hence, if the oxygen concentration can be controlled by the EGR, then the NOx production may be regulated directly, allowing more robust control of the NOx production. (Hereafter this is referred to as direct NOx control.) However, because the NOx sensor response is too slow to detect the NOx concentration transitionally, it is estimated by the NOx soft sensor.

Figure 2 shows the relationships among the NOx concentration, MAF, and the O2 concentration obtained in the experiments. In chart (a), where the MAF is taken as the independent variable, the plots of both the high and low boost pressures exhibit greater variations in NOx and DPM. In contrast, in chart (b), where the O2 concentration is taken as the independent variable, the plots of boost pressures follow nearly the same curve in both NOx and DPM, regardless of the pressure variation, suggesting direct controllability of NOx by the O2 concentration.

![Figure 2](image-url)

Figure 2. Mutual relation of NOx and MAF or O2 concentration. In case of order by MAF, NOx varies by MAP, however in case of order by O2 concentration, NOx does not vary when the MAP changes.
2.3. NO\textsubscript{X} soft sensor

A typical soft sensor employs either a just-in-time model [4] or a neural network-based [5] method. However, these methods are not model based and the factors that influence NO\textsubscript{X} are indistinct. From the viewpoint of practical calibrations, a soft sensor should be constructed so that the effect of each factor can be tuned independently. In this study, an experiment-based soft sensor model is used. Figure 3 shows the NO\textsubscript{X} soft sensor scheme where the dashed red and solid blue lines denote parameters and variables, respectively. The NO\textsubscript{X} soft sensor calculates the NO\textsubscript{X} concentration as shown in Eq. (2):

\[
\psi_{\text{NO}_x} = \psi_{\text{NO}_x,\text{ref}} \cdot C_{\text{O}_2} \cdot C_{\text{SOI}} \cdot C_{\text{RP}} \cdot C_{\text{Tcool}} \cdot C_{\text{Tinm}}
\]  

(2)

where \(\psi_{\text{NO}_x}\) is the NO\textsubscript{X} concentration as a mole fraction. The factors on the right-hand side \(C_{*}\) affect NO\textsubscript{X}, and are called correction factors. In this equation, the subscripts denote

- \(O2\): \(O_2\) concentration
- \(SOI\): Main injection timing
- \(RP\): Rail pressure
- \(Tcool\): Temperature of the cooling water
- \(Tinm\): Temperature of the intake manifold

Each correction factor is described as

\[
\begin{align*}
C_{\text{O}_2} &= \left( \frac{\psi_{\text{O}_2,\text{cyl,ref}}}{\psi_{\text{O}_2,\text{cyl,ref}}} \right)^{a_{\text{O}_2}} \\
C_{\text{SOI}} &= e^{a_{\text{SOI}}(\theta_{\text{SOI}} - \theta_{\text{SOI,ref}})} \\
C_{\text{RP}} &= \left\{ a_{\text{RP}} \cdot \left( P_{\text{rail}} - P_{\text{rail,ref}} \right) + 1 \right\} \\
C_{\text{Tcool}} &= \left\{ a_{\text{Tcool}} \cdot \left( T_{\text{cool}} - T_{\text{cool,ref}} \right) + 1 \right\} \\
C_{\text{Tinm}} &= \left( \frac{T_{\text{inm}}}{T_{\text{inm,ref}}} \right)^{a_{\text{Tinm}}} 
\end{align*}
\]  

(3)

In Eqs. (2) and (3), the variables with subscript the \textit{ref} denote the nominal values under standard atmospheric conditions, while the variables with \(a_{*}\) indicate calibration values when the operation condition differs from the standard condition (i.e., the variable does not affect the calculated value when the state is the same as the nominal condition). Each nominal value (\(*_{,\text{ref}}\)) and calibration value (\(a_{*}\)) can be defined to form a 2D map using engine speed and fuel injection quantity as the parameters.

**Figure 3.** Structure of NO\textsubscript{X} soft sensor.
2.4. Adaptive NO\textsubscript{X} soft sensor

To eliminate the offset in the NO\textsubscript{X} soft sensor, the gain of the offset is compensated compared with the NO\textsubscript{X} hard sensor value. Figure 4 diagrams the proposed adaptive NO\textsubscript{X} soft sensor. SPSA was originally proposed by Spall in 1987 [6] as a very efficient optimization technique.

![Figure 4. Composition of the NO\textsubscript{X} soft sensor using SPSA.](image)

In Eq. (3), each calibration value $a_*$ is rewritten to the adaptation value $a_{\text{SPSA}*}$ by modifying function $f_{\text{comp}*}$ as follows

$$a_{\text{SPSA}*} = a_* \cdot f_{\text{comp}*}(\theta) \quad (4)$$

where, each modifying function $f_{\text{comp}*}$ is described as two-dimensional linear function with three tuning parameters $a_1*$, $a_2*$, and $b_*$, and two engine parameters which are engine speed $N_e$ and fuel injection quantity $q_{\text{fni}}$

$$f_{\text{comp}*} = a_1* \cdot N_e + a_2* \cdot q_{\text{fni}} + b* \quad (5)$$

Since the soft sensor has five calibration factors, the total number of the tuning parameters of the adaptive NO\textsubscript{X} soft sensor is 15, and they are tuned online by SPSA efficiently. For instance, the O\textsubscript{2} calibration value map is tuned as shown in figure 5.

![Figure 5. Adaptation method for calibration map.](image)
Regarding to the online adaptive tuning method using a modified SPSA, it is proposed by the authors [7, 8]. In this study, our modified SPSA is utilized. Figure 5 shows the composition of the adaptive NO\textsubscript{X} soft sensor. The NO\textsubscript{X} soft sensor value $\psi_{\text{NO}_\text{X}, \text{soft}}$ is compared with NO\textsubscript{X} hard sensor value $\psi_{\text{NO}_\text{X}, \text{hard}}$ through the predictor $G_{\text{predict}}$ that predicts the value after the hard sensor delay, and the error $e$ is derived. The loss function $L$ is calculated from the error $e$, and the tuning parameters are updated to $\theta_{k+1}$ by the modified SPSA, then the modifying function $f_{\text{comp}}$ is derived. After that, the adaptation value $\alpha_{\text{SPSA}*}$ is calculated by multiplying $f_{\text{comp}}$ and the calibration value $C_{*}$, then the correction factor $C_{*}$ is derived and the soft sensor value is updated. The above process is sequentially repeated online.

3. SPSA
The modified SPSA is briefly described here. For more details, refer to [7]. The SPSA procedure is in the general recursive stochastic approximation form as shown in Eq. (6):

$$\hat{\theta}_{k+1} = \hat{\theta}_k - a_k \hat{g}_k (\hat{\theta}_k)$$  \hspace{1cm} (6)

where $\hat{\theta}_k$ is the estimated optimization parameter vector, $a_k$ is the update gain, and $\hat{g}_k(\hat{\theta}_k)$ is the estimated value of the gradient for the parameter, which is described as

$$\hat{g}_k (\hat{\theta}_k) = L \left( \hat{\theta}_k + c_k \Delta_k \right)$$

where $L$ is the loss function, $c_k$ is a perturbation gain with a minute positive value to adjust the perturbation, and $\Delta_k$ is a bounded $p$-dimensional random number vector with a symmetric distribution when the expected value is 0 and no element can ever be zero (e.g., a Bernoulli distribution). For example, Eq. (8) shows a random number vector expressed as a random binary sequence

$$\Delta_k = \{1, -1, -1, 1, -1, 1, \ldots\}^T$$  \hspace{1cm} (8)

By choosing $a_k$ and $c_k$ appropriately and iterating Eq. (6) recursively, the estimated optimal parameters converge to an optimal value as a stationary system. The standard SPSA evaluates the loss function twice by perturbing all the tuning parameters simultaneously. In this case, a one-time evaluation SPSA [9] is used. The sum of the squared error is used as the loss function.

4. Experiment
4.1. Engine bench
The adaptive NO\textsubscript{X} soft sensor algorithm was modeled with Simulink and downloaded to a rapid controller prototyping environment. The diesel engine was for a medium truck with a displacement of about 5,200 cc. Table 1 shows the specifications, and figure 8 shows the engine bench.

| Table 1. Engine specifications. |
|---------------------|---------------------|
| **Type**            | **Direct injection, DOHC, IC turbo** |
| Displacement        | 5193 cc             |
| Compression ratio   | 15.5                |
| Maximum power       | 140 kW / 2600 rpm   |
| Maximum torque      | 510 Nm / 1600 rpm   |
| Regulation          | Euro 6              |
Each calibration value \( \alpha \) in Eq. 3 is obtained by calibrating the engine in a standardized environment. To create artificial environments that differ from the calibrated one, the following variations are introduced.

- EGR valve openness: Half of the nominal value (The \( \text{O}_2 \) concentration and intake gas temperature are varied.)
- Main injection timing of fuel: Delay of the crank angle by 2° with respect to the nominal value
- Common-rail pressure: 30 MPa less than the nominal value

To simulate non-adaptation between the engine and the calibration value map due to the deterioration with engine age, variations among engines, and differences in products, each calibration value map is multiplied by 1.5 and the NO\(_X\) value is measured in each of the following cases:

- NO\(_X\) hard sensor (labeled “HS”)
- Environmental variation + calibration map normal (labeled “SS: normal”)
- Environmental variation + calibration map error (labeled “SS: w/o adapt”)
- Environmental variation + calibration map error + SPSA adaptation (labeled “SS: with adapt”)

4.2. Stationary test

The test was carried out at the middle and high engine speed points while changing the amount of fuel injection such that the load was changed stepwise. The upper plot in figure 7 shows the test pattern. The blue and green lines indicate the engine speed trace and the change in the amount of fuel injection, respectively.

The lower plot in figure 7 shows the NO\(_X\) concentration where black solid, red dashed-dotted, green dotted, and blue chain lines indicate the values measured by a hard sensor, a soft sensor without calibration map error, a soft sensor with calibration map error, and an adaptive soft sensor with calibration map error. To make a direct comparison of the hard and soft sensors, the dynamics of each soft sensor response is compensated by the hard sensor delay. In the case of the soft sensor with calibration map error, the value deviates significantly from the hard sensor. Although the error is slightly smaller in the case of the soft sensor without calibration map error, the error is still large. However, the proposed adaptive soft sensor can adapt to appropriately reduce the error.
4.3. Transient test

A WHTC mode test was conducted to confirm the adaptability of the adaptive NO\textsubscript{X} soft sensor using SPSA for transient operations. The WHTC mode, which is an international mode test of the transient operation for exhaust emissions, is a practical operational cycle covering a broad range of conditions (Figure 8). Figure 9 shows the values of NO\textsubscript{X}. Because the WHTC mode test can last as long as 1,800 sec, the chart is divided into 300 sec sections to improve the visibility of the chart.

Conventional soft sensors usually deviate largely from the values of the NO\textsubscript{X} hard sensor (HS) in the region where the NO\textsubscript{X} values fluctuate vigorously, even if there are no errors in the calibration map (SS: normal). If the calibration map contains errors (SS: w/o adapt), the deviation becomes even larger. In contrast, the adaptive NO\textsubscript{X} soft sensor using SPSA (SS: with adapt) adapts considerably to the NO\textsubscript{X} hard sensor, even in the region where the fluctuation of the NO\textsubscript{X} values is substantially large, except for some segments.

Figure 10 shows the deviation from the NO\textsubscript{X} hard sensor as the RMS error, where the data are presented in five-second moving averages of the RMS values weighted by the Hann window function. Although the deviation becomes larger in some segments, the plot shows a considerable adaptation overall. The effect is markedly prominent, especially after 900 seconds.
Figure 9. NO\textsubscript{X} value under WHTC mode test. The black solid line is hard sensor as reference. The red dashed line, green dashed-dotted line and blue dotted line indicates the conventional the soft sensor without calibration map error, the conventional soft sensor with calibration map error, and the proposed adaptive soft sensor with calibration map error, respectively. In the conventional method, in case of calibration map error, deviations become larger. However, the proposed method can follow-up to the hard sensor throughout mode test.
Figure 10. Moving RMS error under WHTC mode test. The errors are calculated multiplying Hann window of 5s period, and running. The black solid line, the red dashed line and the blue dashed-dotted line indicates the conventional soft sensor without calibration map error, the conventional soft sensor with calibration map error, and the proposed adaptive soft sensor with calibration map error, respectively. The proposed method can adapt and reduce the error even though the calibration maps have errors.
5. Conclusion
This study investigates the use of NO\textsubscript{X} soft sensors in the aftertreatment of diesel engines. To eliminate the offset from the NO\textsubscript{X} hard sensor, an adaptive NO\textsubscript{X} soft sensor using SPSA is proposed. The most distinctive feature of the SPSA algorithm is that the calculation only requires that the loss function be determined once or twice per iteration regardless of the number of optimization parameters. In this study, the soft sensor model has five calibration factors, consequently they have 15 tuning parameters, which are simultaneously tuned and updated using SPSA. The adaptability of the proposed method is confirmed using a staircase load test for stationary conditions and WHTC mode test for transient conditions on engine bench. Even if the condition differs significantly from the standard condition, the proposed method adapts appropriately in both cases of stationary and transient conditions. In the future, it is planned to implement the proposed method to direct to the NO\textsubscript{X} control system.

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