An Extended Kalman Filter for NO\textsubscript{x} Sensor Ammonia Cross-Sensitivity Elimination in Selective Catalytic Reduction Applications

Ming Feng Hsieh and Junmin Wang*
Department of Mechanical Engineering
Ohio State University, Columbus, OH 43210

Abstract—Vehicle NO\textsubscript{x} emission regulations are becoming more and more stringent worldwide. A selective catalytic reduction (SCR) system which uses ammonia as the reductant to reduce tailpipe NO\textsubscript{x} emissions is widely adopted by Diesel engine applications. For SCR control, a NO\textsubscript{x} sensor is commonly used to monitor the emissions, however it has been discovered that NO\textsubscript{x} sensors typically are cross-sensitive to the presence of ammonia. Such a feature becomes a critical problem as ammonia slip can be present downstream of a SCR catalyst where the NO\textsubscript{x} sensor is located. To address this issue, an extended Kalman filter (EKF) is designed in this paper to estimate the actual exhaust gas NO\textsubscript{x} concentration and the cross-sensitive factor such that the cross-sensitivity error can be eliminated.

I. INTRODUCTION

With the increasing concerns on energy consumption and environment, including the greenhouse gas emissions, worldwide, Diesel engines have attracted much attention in recent years due to their better fuel efficiency and lower CO\textsubscript{2} emission compared to their gasoline counterparts. However, Diesel engines also feature higher NO\textsubscript{x} emissions which have been tightly restricted by emission regulations worldwide in recent years. It has been studied that the stringent NO\textsubscript{x} emissions regulations in the near future cannot be satisfied by pure engine control alone [21]-[25]. An aftertreatment system is necessary to further reduce tailpipe NO\textsubscript{x} emissions. Among a variety of options, selective catalytic reduction (SCR) is one of the most promising technologies for Diesel engine vehicle applications.

SCR utilizes ammonia as the reductant to convert the NO\textsubscript{x} emission to diatomic nitrogen. Several SCR controllers have been proposed in recent years to control the SCR catalyst ammonia concentration such that the tailpipe NO\textsubscript{x} emission can be minimized [3]-[6]. Among the controllers surveyed in the study of [7], it is widely considered that feedback control is necessary to reduce the NO\textsubscript{x} emissions to an acceptable level and to prevent undesired ammonia slip. Feedback control of SCR requires measurements of tailpipe NO\textsubscript{x} and ammonia concentrations. NO\textsubscript{x} sensors have been available in production for a few years and ammonia sensors for aftertreatment application were recently available from suppliers such as Delphi [8]. An important issue is that many studies have pointed out that NO\textsubscript{x} sensors have significant cross-sensitivity to ammonia [7]-[10]. The ammonia cross-sensitivity can cause overrated tailpipe NO\textsubscript{x} emissions and the closed loop system becomes potentially unstable. Even though the problem is critical for SCR control, not many effective solutions can be found in literature. Most applications adopt the straightforward manner of utilizing a factory provided cross-sensitivity constant to compensate the error based on the sensor model [10]. However, this may not be sufficient especially as the vehicle emission regulations are stringent enough to where consistent and precise measurement of NO\textsubscript{x} concentration is essential. The cross-sensitivity factor can be different between sensors and also can change with time due to sensor aging and environmental variations. By these effects, the conventional correction approach may not work as well as expected. In this paper, with the recently available ammonia sensors, we propose an approach of using an extended Kalman filter (EKF) [1][2][20] to estimate the actual NO\textsubscript{x} concentration and ammonia cross-sensitivity factor such that the NO\textsubscript{x} sensor cross-sensitivity error can be well handled.

The rest of this paper is organized as follows. A brief introduction of the SCR model is presented in the second section. After that, an EKF for the ammonia cross-sensitivity error elimination is designed. Then simulations based on an experimentally-validated full-vehicle simulator are introduced to verify the proposed approach. At the end of the paper, conclusive remarks are summarized.

II. SELECTIVE CATALYTIC REDUCTION (SCR)

A. SCR Operation Principles

The SCR NO\textsubscript{x} reduction mainly includes three processes. In the first process, ammonia is injected upstream of the SCR catalyst as the reductant. In the second process the ammonia inside the catalyst is partially adsorbed on the catalyst surface. And then the adsorbed ammonia can react with NO\textsubscript{x} and convert it to nitrogen molecule and water. A schematic view of SCR operations is shown in Fig. 1.

The dominant chemical reactions and the corresponding reaction rates are briefly introduced below.

1) NH\textsubscript{3} Adsorption/Desorption

The NH\textsubscript{3} inside the SCR catalyst can be adsorbed on the SCR substrate. The adsorbed NH\textsubscript{3} can also be desorbed from the substrate as shown in the following reaction equation.

\[
\text{NH}_3 + \theta \leftrightarrow \text{NH}_3^\theta, \quad (1)
\]

where \(\theta\) is the free catalyst site.

The rate of the NH\textsubscript{3} adsorption/desorption can be expressed by the following equations [11].
\[ R_{ads} = k_{ads} \exp \left( -\frac{E_{ads}}{RT} \right) C_{NH_3}(1 - \theta_{NH_3}), \]  
\[ R_{des} = k_{des} \exp \left( -\frac{E_{des}}{RT} \right) \theta_{NH_3}, \]

where \( R_x \) represent the chemical reaction rates, \( T \) is temperature, \( E \), \( k \), and \( R \) are constants, \( C_x \) represented concentration of species \( x \), and \( \theta_{NH_3} \) is the ammonia surface coverage ratio define by:

\[ \theta_{NH_3} = \frac{M_{NH_3}'}{\theta} \]

\( M_{NH_3}' \) is the mass of ammonia stored in the SCR substrate and \( \theta \) is the ammonia storage capacity.

2) \( NO_x \) Oxidation

Also, at a temperature higher than 450 deg C, the adsorbed \( NH_3 \) can be oxidized to \( NO \) by the following reaction.

\[ NH_3^* + 1.25O_2 \rightarrow NO + 1.5H_2O, \]  
\[ R_{oxi} = k_{oxi} \exp \left( -\frac{E_{oxi}}{RT} \right) \theta_{NH_3}. \]

3) \( NO_x \) Reduction

The adsorbed \( NH_3 \) can then catalytically react with \( NO_x \) to become nitrogen by the following reactions.

\[ 4NH_3^* + 4NO + O_2 \rightarrow 4N_2 + 6H_2O, \]  
\[ 2NH_3^* + NO + NO_2 \rightarrow 2N_2 + 3H_2O, \]  
\[ 4NH_3^* + 3NO_2 \rightarrow 3.5N_2 + 6H_2O. \]

Because more than 90% of the Diesel engine-out exhaust \( NO_x \) is usually composed of \( NO \) [12]. Assuming there is no DOC/DPF presented upstream of the SCR catalyst, reaction in Eq. (7) is considered the dominant one in \( NO_x \) reductions. The reaction rate is described below [6]:

\[ R_{red} = k_{red} \exp \left( -\frac{E_{red}}{RT} \right) C_{NO} \theta_{NH_3}. \]

In case a DOC/DPF is used upstream of the SCR catalyst, fraction of \( NO_2 \) inside \( NO_x \) can be increased significantly. With this situation the reaction of Eq. (8), which is much faster than the reaction in Eq. (7), should be considered.

\[ \dot{C}_{NO} = \theta(R_{oxi} - R_{red}), \]  
\[ \dot{\theta}_{NH_3} = R_{ads} - R_{des} - R_{red} - R_{oxi}, \]  
\[ \dot{C}_{NH_3} = \theta(R_{des} - R_{ads}). \]

Such dynamic equations can be used to develop a SCR model using the continuous stirred tank reactor (CSTR) approach and mass conservation law. Different SCR models for vehicle applications have been proposed in the literature [11]-[14]. In this paper we adopted the model presented in [11]. The nonlinear model in state-space form is shown in Eq. (14).

\[
\begin{bmatrix}
\dot{C}_{NO} \\
\dot{\theta}_{NH_3} \\
\dot{C}_{NH_3}
\end{bmatrix} =
\begin{bmatrix}
-C_{NO} (\theta_{red} \theta_{NH_3} + \frac{r}{T}) + r_{NH_3-oxi} \theta_{NH_3} \\
-\theta_{NH_3} (r_{ads} C_{NH_3} + r_{des} C_{NO} + r_{oxi}) + r_{ads} C_{NH_3} \\
r_{ads} + \theta_{ads} \theta_{NH_3}
\end{bmatrix} + \begin{bmatrix}
r_{oxi} \\
0 \\
0
\end{bmatrix},
\]

where \( r_x = k_x e^{-\frac{E_x}{RT}} \); \( x = ads, des, oxi, red; C_{NO} \) and \( C_{NH_3} \) are the tailpipe \( NO_x \) and ammonia concentrations; \( C_{NH_3, in} \) is the pre-SCR ammonia concentration controlled by the SCR controller; and \( C_{NO, in} \) is the engine exhaust \( NO_x \) concentration.

III. EXTENDED KALMAN FILTER FOR \( NO_x \) SENSOR AMMONIA-SENSITIVITY ESTIMATION

A. \( NO_x \) Sensor Cross-Sensitivity against Ammonia

A typical setup of the SCR and the corresponding sensors is shown in the figure below.

![Figure 2. Architecture of SCR and the corresponding sensors.](image)

It has been known that \( NO_x \) sensors are cross-sensitive against the presence of ammonia. The measurement \( C_{NO, sen} \) from the \( NO_x \) sensor can be modeled by the superposition of \( NO_x \) on ammonia concentration as below [3].

\[ C_{NO, sen} = C_{NO} + K_{cs} C_{NH_3}, \]

where \( K_{cs} \) is the cross-sensitivity factor, \( C_{NO} \) is the actual \( NO_x \) concentration, and \( C_{NH_3} \) is the (actual) ammonia concentration in the exhaust gas.

It can be seen from Figure 2 that the pre-SCR \( NO_x \) sensor is not affected by the ammonia cross-sensitivity since it is placed upstream of the urea injector. However, the post-SCR \( NO_x \) sensor is subjected to ammonia slip and measurement error caused by the ammonia-sensitivity,
\( K_{cs}C_{\text{NH}_3} \). This not only hampers the effectiveness of the NOx sensor, but also makes the SCR controller potentially unstable and can induce unnecessary urea cost. With the cross-sensitivity, it is possible that the more ammonia injected, the higher the NOx reading from the post-SCR NOx sensor, because of the higher ammonia slip.

A common approach to address this problem is to predict the actual NOx concentration using the sensor model in Eq. (15) and the corresponding ammonia measurement and a factory provided cross-sensitivity factor \( K_{cs} \). However, it is believed that the cross-sensitivity factor has variance between sensors, and slowly time-varying bias can be expected as the environment changes and the sensor ages. An inaccurate cross-sensitivity factor can cause serious NOx concentration measurement error and an observer must be designed to estimate the actual value.

As the cross-sensitivity factor changes slowly with time, it is not easy to develop a model to predict this variation, and a conventional model-based observer is hard to be designed to estimate this value. To better address this problem, we propose the idea of using an extended Kalman filter (EKF) to estimate the value based on an approximated model and the stochastic process calculation.

### B. EKF Design for NOx Cross-Sensitivity Elimination

1) Extended Kalman Filter (EKF)

Kalman filter is well-known as an efficient recursive filter that can optimally estimate the state of a linear dynamic system from a series of noisy measurements [20]. For nonlinear systems, extended Kalman filter has been developed and validated by many studies to be effective in real applications [15]-[17]. Unlike model-based observers which heavily rely upon plant models and measurements, a specific feature of a Kalman filter is that it finds the stochastic relations between model predictions and sensor measurements, and then estimates system states in an optimal approach. By utilizing this feature of the Kalman filter, a slowly time-varying state can be modeled as a constant and then be estimated by comparing the sensor biases from gyroscopes and accelerometers. In this study, the cross-sensitivity factor \( K_{cs} \) in Eq. (15) is also a slowly time-varying state. A general formulation of EKF is presented below.

The nonlinear system to be dealt with by an EKF is generally expressed in the following form:

\[
x(k) = f(x(k-1), u(k)) + w(k),
\]

\[
z(k) = h(x(k)) + v(k),
\]

where \( w(k) \) and \( v(k) \) are the process and observation noises with zero-mean multivariate Gaussian noise with covariance of \( Q(k) \) and \( R(k) \).

By the model described in Eq. (16) and Eq. (17), an EKF estimates the states by two steps: prediction and update. In the prediction step, the state vector \( x \) and the error covariance matrix \( P \) are predicted as follows:

\[
x(k|k-1) = f(x(k-1|k-1), u(k)), \quad (18)
\]

\[
P(k|k-1) = F(K)P(k-1|k-1)F(K)^T + Q(k), \quad (19)
\]

where \( F \) is the Jacobian matrix of the state function \( f \).

Then in the update step, the predicted system states \( x(k|k-1) \) and error covariance matrix \( P(k|k-1) \) are updated by comparing them to the measurement \( z(k) \).

Based on the assumption that the noises are zero-mean Gaussian distribution, the optimal Kalman gain \( K(k) \) and the estimated value \( x(k) \) can be calculated by the following equations:

\[
y(k) = z(k) - h(x(k|k-1)), \quad (20)
\]

\[
S(k) = H(k)P(k|k-1)H(k)^T + R(k), \quad (21)
\]

\[
K(k) = P(k|k-1)H(k)^T S(k)^{-1}, \quad (22)
\]

\[
x(k|k) = x(k|k-1) + K(k)y(k), \quad (23)
\]

\[
P(k|k) = (I - K(k)H(k))P(k|k-1) \quad (24)
\]

where \( H \) is the Jacobian matrix of the output function \( h \).

### 2) EKF for Cross-Sensitivity Factor and NOx Concentration Estimations

Because the cross-sensitivity factor \( K_{cs} \) in Eq. (15) is assumed to be a slowly time-varying variable, it can be modeled by the following equation:

\[
\dot{K}_{cs} = 0. \quad (25)
\]

And based on the SCR model in Eq. (14), the NOx concentration is modeled by the following equation:

\[
\hat{C}_{\text{NO}} = -\hat{C}_{\text{NO}} \left( \theta r_{\text{red}} \theta_{\text{NH}_3} + \frac{F}{V} \right) + r_{\text{oxi}} \theta_{\text{NH}_3} + \frac{F}{V} C_{\text{NO}_{\text{sen,in}}} \quad (26)
\]

where \( C_{\text{NO}_{\text{sen,in}}} \) is measured by the upstream NOx sensor which is not affected by the ammonia cross-sensitivity under the assumption \( C_{\text{NO}_{\text{sen,in}}} = C_{\text{NO}} \). \( V \) is a constant, \( F \), \( r_{\text{NH}_3,\text{oxi}} \), and \( r_{\text{red}} \) are available from measurements and corresponding models, \( \theta \) is assumed to be a known and temperature-dependent variable, and \( \theta_{\text{NH}_3} \) is the ammonia surface coverage ratio which is estimated by the observer developed in [18].

By the above models, the prediction equation in discrete form is obtained below.

\[
x(k|k-1) = \begin{bmatrix} \hat{C}_{\text{NO}}(k|k-1) \\ \hat{C}_{\text{NO}}(k|k-1) \\ \hat{C}_{\text{NO}}(k|k-1) \end{bmatrix} = \begin{bmatrix} \hat{C}_{\text{NO}}(k|k-1) + \Delta t \hat{C}_{\text{NO}}(k|k-1) \\ \hat{C}_{\text{NO}}(k|k-1) + \Delta t \hat{C}_{\text{NO}}(k|k-1) \end{bmatrix} \quad (27)
\]

where \( \Delta t \) is the EKF updating period. The EKF measurement is the post-SCR NOx sensor reading \( C_{\text{NO}_{\text{sen}}} \) which can be modeled as:

\[
z(k) = C_{\text{NO}_{\text{sen}}}(k) = C_{\text{NO}}(k|k-1) + \hat{R}_{cs}(k|k-1) \quad (28)
\]
where $C_{NH_3}$ is the ammonia concentration reading from the post-SCR ammonia sensor which is assumed to be accurate enough.

Based on the prediction and measurement equations of Eq. (27) and Eq. (28), the extended Kalman filter for the estimations of post-SCR NO$_x$ concentration, $C^*_NO$, and the sensor cross-sensitivity factor, $K_{CS}$, can be constructed according to Eq. (18) to Eq. (24).

### IV. SIMULATION RESULTS

Simulations of the proposed EKF NO$_x$ concentration estimator were done using an experimentally-validated full vehicle simulator cX-Emission developed by the Center for Automotive Research at the Ohio State University [19]. Normally (Gaussian) distributed noises with zero mean values were imposed to all the sensor measurements. The simulations were based on the FTP75 test cycle. Vehicle speed, pre-SCR NO$_x$ concentration, exhaust flow rate, and the exhaust temperature during the cycle are presented in Figure 3. Notice that to feature the presence of NO$_x$ sensor ammonia cross-sensitivity, more-than-normal amount of urea was injected during the simulation to have extra high tailpipe ammonia slip, also higher load was imposed to the simulated vehicle in order to have more NO$_x$ emissions.

Two cases are presented in the following simulation results. The first case assumes the cross-sensitivity factor to be a constant during the test cycle, and the EKF estimates this value with an initial value of zero which is different from the value in the model. The second case imposed a slowly time-varying cross-sensitivity factor. The estimation also started from an initial value of zero, different from the model value. Practically, considering sensor aging, the time-varying effect is unnoticeable from a single FTP75 cycle which is the situation in the first case. On the other hand, for some sensors, the cross-sensitivity factor can change with environment. In this case, noticeable variation could be observed during the time period of a test cycle, which is imitated in the second case.

**A. Case 1: Constant Cross-Sensitivity Factor during a Cycle**

Figure 4 shows the comparisons of model predicted post-SCR ammonia concentration, post-SCR NO$_x$ sensor reading, model predicted NO$_x$ concentration, EKF estimated NO$_x$ concentration, and estimated cross-sensitivity factor. The cross-sensitivity factor was selected to be 0.5 as a constant during the test cycle. As seen in Figure 4, the post-SCR NO$_x$ sensor reading is always higher than the actual NO$_x$ concentration due to the presence of ammonia.

**Figure 4. Comparisons of ammonia concentration, NO$_x$ measurement, model predicted NO$_x$ concentration, and estimated NO$_x$ concentration calculated by EKF.**

**Figure 5. Zoom-in on beginning porting of the Figure 4.**

Figure 5 shows the first 200 seconds of the test cycle which offers a better presentation. It can be seen that the predicted NO$_x$ concentration converged to the true value as the estimated cross-sensitivity factor approached its true value. It is clear that the NO$_x$ estimation is robust to the presence of ammonia.

**Figure 6. Comparisons of errors of post-SCR sensor measurement and estimated NO$_x$ concentration and the corresponding ammonia concentration.**

Figure 6 shows the comparisons of errors between the actual NO$_x$ concentration and the NO$_x$ sensor reading and NO$_x$ concentration after the EKF-based correction. The
cross-sensitivity of the NOx sensor against ammonia can be clearly seen. Also we can see that the EKF significantly reduced the cross-sensitivity error.

Figure 7 shows the comparison between the true cross-sensitivity factor in the model and the predicted value. It can be seen that the estimated value converged to the actual value fairly well.

There exist some deviations at the time regions around the 200th second and the 1700th second which also caused higher NOx estimation error as can be observed in Figure 6. These are due to the fact that the vehicle was quickly accelerated to high speeds as can be seen in the speed profile in Figure 3. At these moments, the temperature, exhaust gas flow rate, and NOx emissions, together with ammonia injection, were increased significantly such that the system was hardly approximated by the linearized models in the EKF, i.e. Eq. (18), Eq. (21), and Eq. (24). Since the model cannot capture the real dynamics very well, higher estimation errors were presented. However, the errors caused by these variations are still acceptable. The situation can be improved by increasing the EKF updating rate, i.e. decrease $\Delta t$ in Eq. (27), if computation capability is allowed.

B. Case 2: Slowly Time-Varying Cross-Sensitivity Factor

In this case the cross-sensitivity factor is modeled as a time-varying variable during the cycle as shown in Figure 8 and Figure 10. In Figure 8 we can see, because of the time-varying cross-sensitivity factor, the post-SCR NOx sensor reading not only changed with NOx concentration and ammonia concentration but was also affected by the factor variation. However, as expected, the estimated NOx concentration can still track the actual value very well.
addressed in this paper. It has been studied that the cross-sensitivity of NO\textsubscript{x} sensor can raise a serious issue for Diesel engine SCR system control because ammonia is used as the reductant and the presence of tailpipe ammonia slip can induce significant measurement error on the post-SCR NO\textsubscript{x} sensor. This problem was generally handled by an experimental model to predict the cross-sensitive value in an open-loop fashion which is not a reliable manner when NO\textsubscript{x} emissions have to be monitored precisely. An extended Kalman filter-based estimation approach was proposed in this paper. The method utilized the stochastic character of EKF and an approximate cross-sensitivity factor model to estimate the actual NO\textsubscript{x} concentration and cross-sensitivity factor. Simulation results based on the FTP75 test cycle verified the approach of being able to accurately eliminate the cross-sensitivity error caused by the presence of ammonia and to well predict the NO\textsubscript{x} concentration and cross-sensitivity factor.

ACKNOWLEDGMENT

The authors would like to thank the partial financial support provided to this research by the members of The Ohio State University Center for Automotive Research (OSU-CAR) Industrial Consortium.

REFERENCES


