An extended Kalman filter for input estimations in diesel-engine selective catalytic reduction applications

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ABSTRACT

Nowadays the legislative regulation on emissions of Diesel engines is stringent such that an after-treatment system is necessary. To reduce vehicle NO_x emission, a selective catalytic reduction (SCR) system is widely used for Diesel-engine applications. In the SCR system, the gaseous ammonia plays a significant role which is utilized as the reduction to eliminate the NO_x emission. To facilitate the NO_x reduction, a NO_x sensor and an ammonia sensor placed before the SCR catalyst are a good strategy. However, physical sensors would increase the system cost and diagnosis challenge. To reduce the number of physical sensors, in this paper, observers are designed with the assist of extended Kalman filter (EKF) to estimate the NO_x or ammonia concentrations before the SCR catalyst. Simulation results show that the designed observers based on EKF can achieve the prescribed objectives quite well.

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1. Introduction

During past decades, the concerns over energy shortages and environmental pollution problems have been growing. A phenomenon is that more and more researchers pay attention to Diesel engines due to their excellent fuel efficiency and lower green house emissions compared to counterparts of gasoline engines [1]. However, the Diesel-engine cylinder temperature is relatively high, which leads to high NO_x emissions. To avoid the NO_x pollution, increasingly stringent emission regulations have been enacted by the government in recent years[2]. Many efforts have been paid to deal with the high-NO_x emission problems. Among which the combustion control and aftertreatment systems are widely studied. It has been shown that only the combustion control cannot achieve the stringent emission regulations [3–5]. Consequently, an aftertreatment system becomes essential for the NO_x issue. Among many aftertreatment techniques, the lean NO_x traps [6] and selective catalytic reduction (SCR) systems [7–10] are the most common methods. Since the lean NO_x trap would affect the diesel engine fuel economy, the SCR system is the most promising technique for the Diesel-engine vehicle applications.

The SCR system makes use of ammonia as the reductant to convert the NO_x emissions to diatomic nitrogen and waters. In an SCR system, the urea injection is the only one input control. Thus, the urea dosage control is critical for the system operation. If the

liquid urea is over dosed than the NO_x emission, the gaseous ammonia would slip into the tailpipe. Since the gaseous ammonia is harmful to the environment, the tailpipe ammonia slip should be reduced as much as possible. On the other hand, to achieve the maximum efficiency of NO_x conversion, the adequate urea injection is necessary [11,12]. Therefore, an SCR dosage control which can minimize the NO_x emissions and tailpipe ammonia slip is crucially important. Many studies on the urea dosage control can be seen in [13,14].

In general, the NO_x concentration, the NH_3 concentration, and the ammonia coverage ratio are considered as the states in the control-oriental SCR model. Furthermore, the input concentrations of ammonia and NO_x are important signals to determine the NO_x reduction efficiency and regulate the urea injection rate [15]. To obtain these information, two ammonia sensors and two NO_x sensors are used to measure the input and output concentrations. However, the physical commercial sensors are costly, which would increase the SCR integration cost. Inspired by the confliction, we aim to design an observer based on the extend Kalman filter (EKF) [16–18] to estimate the ammonia and NO_x inputs, respectively.

In this paper, we propose a technique by utilizing the EKF to estimate the actual input concentration of ammonia or NO_x with only three concentration sensors (not include the temperature sensor). Two cases are considered as below: (1) *Estimate the ammonia input concentration*: In this case, two NO_x sensors are placed at the entrance of SCR device and the tailpipe respectively, and one ammonia sensor located at the tailpipe. Therefore, the output concentrations of ammonia and NO_x are available. Besides, the input concentration of NOx is known as well. Then, we aim to

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derive the ammonia input concentration through the EKF approach. (2) *Estimate the NO$_x$ input concentration*: In this case two ammonia sensors are placed at the entrance of SCR device and the tailpipe, respectively, and one NO$_x$ sensor located at the tailpipe. Similarly, we aim to get the ammonia input concentration.

The rest of this paper is organized as follows. A concise introduction of the SCR reaction model is shown in Section 2. Then an EKF model for input estimation is designed in Section 3. In Section 4 the simulation results are presented to verify the proposed technique. Section 5 concludes this paper.

2. Selective Catalytic Reduction (SCR)

2.1. SCR operation principle

The main operation of an SCR system can be seen in Fig. 1. In the SCR system, NO$_x$ reduction chiefly involves three parts. First, 32.5% aqueous urea solution is injected before the SCR catalyst can, and urea solution is converted into ammonia through certain number of processes including the evaporation of urea-solution, thermal decomposition of urea, and the hydrolyzation of isocyanic acid. Then, ammonia flow into upstream of the SCR device to deoxygenize NO$_x$. Second, the ammonia is partly adsorbed on the surface of catalyst. Third, the adsorbed ammonia catalytically reacts with NO$_x$ and changes it to nitrogen and water [19].

The primary chemical reactions and relevant reaction rate formulas [20,21] go as follows:

(1) *Urea evaporation*: In the first part of urea-to-ammonia, the urea solution which is in the form of droplets evaporate into the solid phase of urea under the ideal situation [22]. The reaction is shown as below

$$NH_2 - CO - NH_2(liquid) \rightarrow NH_2 - CO - NH_2^* + 6.9H_2O, \quad (1)$$

where $NH_2 - CO - NH_2^*$ represents the solid phase of urea.

(2) *Thermal decomposition of pure urea*: Then, the pure urea is decomposed into equimolar amounts of isocyanic acid and ammonia in the condition with a high exhaust gas temperature. The reaction is represented as below

$$NH_2 - CO - NH_2^* \rightarrow HNCO + NH_3. \quad (2)$$

(3) *Isocyanic acid hydrolyzation*: In this part, the isocyanic acid hydrolyzes before the entrance of SCR system. The reaction is represented as follows:

$$HNCO + H_2O \rightarrow NH_3 + CO_2. \quad (3)$$

(4) *Adsorption/Desorption*: The NH$_3$ on the catalyst surface can adsorb on the SCR substrate, and the adsorbed ammonia can be represented as NH$_3^*$. The adsorbed NH$_3$ can also be desorbed from the SCR substrate. So the reaction is a reversible reaction which is shown as follows:

$$NH_3 + \theta_{free} \rightleftharpoons NH_3^*, \quad (4)$$

where θ_{free} is the free SCR catalyst site.

The rate of the reversible reaction is represented by following equations [23]:

$$R_{ad} = K_{ad} \exp\left(-\frac{E_{ad}}{RT}\right) C_{NH_3}(1 - \theta_{NH_3}), \quad (5)$$

$$R_{de} = K_{de} \exp\left(-\frac{E_{de}}{RT}\right) \theta_{NH_3}, \quad (6)$$

where R_x expresses the rate of the chemical reaction, T represents temperature, E, K, and R, are constants, C_x denotes concentration of sort x, and θ_{NH_3} is the ammonia surface coverage ratio which is defined by
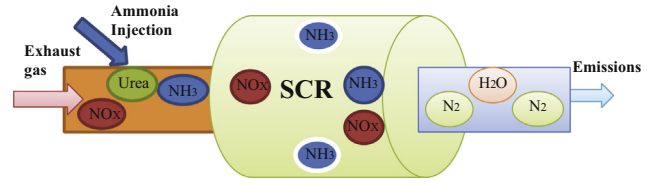

Fig. 1. Schematic diagram of SCR system.
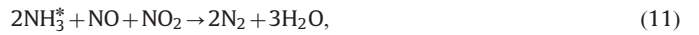
$$\theta_{NH_3} = \frac{M_{NH_3}^*}{\Theta}, \quad (7)$$

where $M_{NH_3}^*$ is the mole number of ammonia garnered in the SCR substrate and Θ represents the ammonia storage capacity.

(5) *NH$_3$ oxidation*: When temperature is higher than 450 °C, the adsorbed NH$_3$ is oxidation to NO. The reaction equation and reaction rate are shown as follows:

$$NH_3^* + 1.25O_2 \rightarrow NO + 1.5H_2O, \quad (8)$$

$$R_{ox} = K_{ox} \exp\left(-\frac{E_{ox}}{RT}\right) \theta_{NH_3}. \quad (9)$$

(6) *NO$_x$ reduction*: The dominant reduction reactions are shown by the following chemical equations:

$$4NH_3^* + 4NO + O_2 \rightarrow 4N_2 + 6H_2O, \quad (10)$$

$$2NH_3^* + NO + NO_2 \rightarrow 2N_2 + 3H_2O, \quad (11)$$

$$4NH_3^* + 3NO_2 \rightarrow 3.5N_2 + 6H_2O. \quad (12)$$

Research has shown that the proportion of NO in total Diesel-exhaust NO$_x$ is more than 90%. Therefore, the reaction in (10) is regarded as the dominant reaction in NO$_x$ reduction processes. The reduction rate is expressed as follows:

$$R_{re} = K_{re} \exp\left(-\frac{E_{re}}{RT}\right) C_{NO}\theta_{NH_3}. \quad (13)$$

2.2. SCR model

On the basis of molar balance and the law of conservation of mass, the dynamic equation of SCR system can be wrote as follows [21]:

$$\dot{C}_{NO} = \Theta(R_{ox} - R_{re}), \quad (14)$$

$$\dot{\theta}_{NH_3} = R_{ad} - R_{de} - R_{re} - R_{ox}, \quad (15)$$

$$\dot{C}_{NH_3} = \Theta(R_{de} - R_{ad}). \quad (16)$$

Assuming that the catalyst is a Continuously Stirred Tank Reactor (CSTR), the SCR model can be developed with these dynamic equations, the law of mass conservation, and the reaction rates mentioned in Eqs. (5), (6), (9) and (13). Though, there are also many other outstanding SCR models for the SCR system of Diesel engine [24–26], to avoid complicated computations from EKF, the sufficient model shown in [21] is adopted. The nonlinear state model is developed as shown in the following equation:

$$\begin{bmatrix} \dot{C}_{NO} \\ \dot{\theta}_{NH_3} \\ \dot{C}_{NH_3} \end{bmatrix} = \begin{bmatrix} -C_{NO}(\Theta r_{re}\theta_{NH_3} + \frac{F}{V}) + r_{ox}\Theta\theta_{NH_3} \\ -\theta_{NH_3}(r_{ad}C_{NH_3} + r_{de} + r_{re}C_{NO} + r_{ox}) + r_{ad}C_{NH_3} \\ -C_{NH_3}\left[\Theta r_{ad}(1 - \theta_{NH_3}) + \frac{F}{V}\right] + \Theta r_{de}\theta_{NH_3} \end{bmatrix}$$
$$+ \begin{bmatrix} 0 \\ 0 \\ \frac{F}{V} \end{bmatrix} C_{NH_3,in} + \begin{bmatrix} \frac{F}{V} \\ 0 \\ 0 \end{bmatrix} C_{NO,in}, \quad (17)$$

where $r_x = K_x \exp\left(-\frac{E_x}{RT}\right)$; $x = ad, de, ox, re$; C_{NO} and C_{NH_3} are the NO$_x$ and ammonia concentrations; $C_{NH_3,in}$ represents the entrance ammonia concentration controlled by the SCR controller; $C_{NO,in}$