Neurocomputing 205 (2016) 329–335

Contents lists available at ScienceDirect

Neurocomputing

journal homepage: www.elsevier.com/locate/neucom

Adaptive unscented Kalman filter for input estimations in Diesel-engine selective catalytic reduction systems

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ARTICLE INFO

Article history:
Received 25 December 2015
Received in revised form
10 March 2016
Accepted 28 March 2016
Communicated by D. Zhang
Available online 11 May 2016

Keywords:
Input estimations
Adaptive unscented Kalman filter
Diesel-engine
Selective catalytic reduction (SCR) system

ABSTRACT

To tackle the challenge of more and more stringent emission regulations, a selective catalytic reduction (SCR) system is widely used all over the world in Diesel-engine applications. In SCR system, input states may be indispensable for onboard diagnostic strategy. Conventionally, the NO_x and ammonia input informations are measured by several sensors, however, physical sensors are too costly for application. Besides, sensors would also increase the burden of diagnosis. Inspired by this problem, in this paper, an adaptive unscented Kalman filter (AUKF) is designed to estimate the input concentrations, due to the excellent capacity to deal with nonlinear system and calculate the noise covariance matrices online. Go a step further, the physical sensors can be replaced by the AUKF-based observer. Simulation results through the vehicle simulator cX-Emission show that the performance of observer based on AUKF is outstanding, and the estimation error is very small.

1. Introduction

In recent years, diesel engines have got more attentions due to their better fuel economy, larger torque supply capabilities and lower carbon dioxide emission compared with gasoline counterparts [1]. However, there are also some other disadvantages of Diesel-engine puzzled researchers, such as high particulate matter (PM) and high NO_x emission. To meet the increasingly stringent emission regulations enacted by the governments, a series of aftertreatment systems are proposed in the Diesel-engine applications [2,3]. Among these aftertreatment systems, the diesel oxidation catalyst (DOC) is used to oxidize the hydrocarbon and carbon monoxide. The diesel particulate filter (DPF) is used to capture the PM. The SCR system is utilized to convert NO_x emission to nitrogen. According to many researches, the SCR system would be the most efficient and promising aftertreatment component for the Diesel-engine powered applications resulting from their better fuel economy and NO_x conversion efficiency [4,5,25].

According to the SCR operation principle, ammonia is utilized to convert the NO_x emission into water and diatomic nitrogen [5]. As the urea injection is the only one control input, the urea dosing control is essential. It infers from many researches that the NO_x concentration, the ammonia concentration, and the ammonia coverage ratio are regarded as the most important states in the control-oriented SCR model [6–8]. In the commercial SCR system, the NO_x and ammonia concentration can be obtained by the current sensory technologies. Generally, two NO_x sensors and two ammonia sensors are needed to measure the input concentration and output concentration respectively [9]. However, the commercial sensors are usually costly, which would add to the overall cost of the SCR system. Besides, too many sensors would also increase the diagnostic burden [10]. Motivated by such needs, a novel observer is designed to estimate the input concentrations in this paper.

The input estimations have attracted a lot of investigations in the past decade. The author in [11] used an EKF observer to estimate the input NO_x concentration and ammonia concentration respectively. In that paper, the comparisons between actual value and input estimations proved that the designed observer can work well to replace physical sensors. While, the EKF algorithm processes the nonlinear system by linearizing the nonlinear model, which would lead to linearization error. What is more, in this algorithm, we need to calculate Jacobian matrices, which would also burden the computational load. The author in [12] adopted the high-gain observer to estimate ammonia coverage ratio and input simultaneously. This method can estimate the different states, and the comparisons represent the performance of the designed observer is outstanding. However, the process and measurement noise were not considered in this work. Actually, the process and measurement noise would be variable during the test cycle, which may influence the estimation. The author in [13] proposed a method to design observer for

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http://dx.doi.org/10.1016/j.neucom.2016.03.065
0925-2312/

Takagi–Sugeno models which are usually used to approximate nonlinear systems. This method employs a series of linear subsystems to approximate a nonlinear system. However, it is difficult to compute the desired solution when there are too many subsystems. Therefore, the designed method is only adopted to simple nonlinear systems [14–18].

In this paper, we focus on the input observer design by using an adaptive unscented Kalman filter. For nonlinear system, if the model is not accurate enough, then the UKF algorithm is considered more suitable than the EKF to do the state estimation [19]. Besides, to address the problem resulted from the variation of process and measurement noise, we proposed an approach through the AUKF to estimate the input concentration. The AUKF can also simplify the selection process of noise covariance matrices [20]. The rest of the paper is organized as follows. In Section 2, the operation principle and SCR model are proposed. In Section 3, the AUKF algorithm is described. In Section 4, simulation results are depicted to validate the performance of the designed observer. Section 5 is the conclusion of this paper.

2. Selective catalytic reduction (SCR)

2.1. SCR operation principle

The main operation of an SCR system is described in Fig. 1. In the SCR system, NO_x reduction procedure is mainly divided into three parts. The first step is urea-to-ammonia conversion. Then the conversion involves three parts which includes urea-solution evaporation, thermal decomposition of solid phase urea, and the hydrolyzation of isocyanic acid. The second step is adsorption of ammonia on the catalyst surface. At last, the third step is the catalytical reaction of adsorbed ammonia and NO_x [21].

The primary chemical reactions and relevant reaction rates are summarized as follows [22]:

(1) *Adsorption/desorption*: Once the ammonia enter into the SCR device, it can adsorb on the surface of catalyst. Meanwhile, the adsorbed ammonia can also be desorbed from the catalyst surface, thus, the reaction is a reversible reaction which is represented in the following:

$$NH_3 + \theta_{free} \rightleftharpoons NH_3^*, \tag{1}$$

where θ_{free} denotes the free SCR catalyst substrate site, and NH_3^* refers to the adsorbed ammonia on the SCR catalyst surface.

The rates of the reaction are represented by following equations respectively:

$$R_{ad} = K_{ad} \exp\left(-\frac{E_{ad}}{RT}\right) C_{NH_3}(1-\theta_{NH_3}), \tag{2}$$

$$R_{de} = K_{de} \exp\left(-\frac{E_{de}}{RT}\right) \theta_{NH_3}, \tag{3}$$

in which R_x denotes the rates of the chemical reactions, T represents reaction temperature, E, K, and R, are reaction constants, C_x refers to the concentration of sort x, and θ_{NH_3} expresses the ammonia surface coverage ratio which can be defined by:

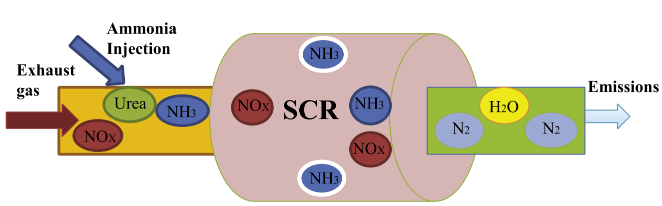

Fig. 1. Schematic diagram of SCR system.

$$\theta_{NH_3} = \frac{M^*_{NH_3}}{\Theta}, \tag{4}$$

where $M^*_{NH_3}$ expresses the mole number of ammonia adsorbed in the SCR substrate and Θ denotes the catalyst ammonia storage capacity.

(2) *NH_3 oxidation*: The adsorbed NH_3 would be oxidated to NO, if temperature is higher than 450 °C. The reaction equation and the reaction rate are presented as below:

$$NH_3^* + 1.25O_2 \rightarrow NO + 1.5H_2O, \tag{5}$$

$$R_{ox} = K_{ox} \exp\left(-\frac{E_{ox}}{RT}\right) \theta_{NH_3}. \tag{6}$$

(3) *NO_x reduction*: NO_x reduction reactions are the most important part in the SCR system. The dominate reactions are proposed as follows:

$$4NH_3^* + 4NO + O_2 \rightarrow 4N_2 + 6H_2O, \tag{7}$$

$$2NH_3^* + NO + NO_2 \rightarrow 2N_2 + 3H_2O, \tag{8}$$

$$4NH_3^* + 3NO_2 \rightarrow 3.5N_2 + 6H_2O. \tag{9}$$

Among the NO_x emission, the proportion of NO almost reaches 90%. Besides, the reaction speed of Eq. (7) is very fast. Therefore, the reaction (7) can be regarded as the dominate reaction. The reaction rate is presented as below:

$$R_{re} = K_{re} \exp\left(-\frac{E_{re}}{RT}\right) C_{NO} \theta_{NH_3}. \tag{10}$$

2.2. SCR model

In this work, we assume that the catalyst is a Continuously Stirred Tank Reactor (CSTR). Considering the chemical reactions proposed above, the law of mass conservation and molar balance, the SCR model can be built [23]. Generally, four states or five states in the model would result in a more accurate estimation of the actual SCR system, as one more variable can describe the system better. However, if we select four-state or five-state model, more sensors are needed in the observer design. In addition, the more states would increase the difficulty of modeling and computing [24]. Therefore, a three-state model is selected in this paper. The SCR state model is built as follows, which is validated through many aftertreatment experiments [22]:

$$\begin{bmatrix} \dot{C}_{NO} \\ \dot{\theta}_{NH_3} \\ \dot{C}_{NH_3} \end{bmatrix} = \begin{bmatrix} -C_{NO}\left(\Theta r_{re}\theta_{NH_3} + \frac{F}{V}\right) + r_{ox}\Theta\theta_{NH_3} \\ -\theta_{NH_3}(r_{ad}C_{NH_3} + r_{de} + r_{re}C_{NO} + r_{ox}) + r_{ad}C_{NH_3} \\ -C_{NH_3}\left[\Theta r_{ad}(1-\theta_{NH_3}) + \frac{F}{V}\right] + \Theta r_{de}\theta_{NH_3} \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ \frac{F}{V} \end{bmatrix} C_{NH_3,in} + \begin{bmatrix} \frac{F}{V} \\ 0 \\ 0 \end{bmatrix} C_{NO,in}, \tag{11}$$

where $r_x = K_x \exp(-\frac{E_x}{RT})$; $x = ad, de, ox, re$; C_{NO} and C_{NH_3} denote the exhaust NO_x and ammonia concentration; $C_{NH_3,in}$ is the input ammonia concentration controlled by the SCR controller; $C_{NO,in}$ refers to Diesel-engine exhaust NO_x concentration; F represents exhaust gas flow rate; V describes the SCR device catalyst volume.

3. Adaptive unscented Kalman filter for input estimations

In the SCR system, input concentrations, state parameter and output concentrations are needed to design a suitable controller [25]. In general, two ammonia sensors, two NO_x sensors and a temperature sensor are located in the system to measure the prerequisite parameter. The schematic presentation of SCR system