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Estimation and adaptive nonlinear model predictive control of selective catalytic reduction systems in automotive applications

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ABSTRACT

The demands of high NO_x conversion efficiency and low tailpipe ammonia slip for urea-based selective catalytic reduction (SCR) systems have been substantially increased in the past decade, as NO_x emission legislations for Diesel engines are becoming more stringent than ever before. Since catalyst aging has a significant impact on SCR performance, robust and adaptive SCR control has been preferred for degraded SCR systems to realize emission control objectives. The purpose of this paper is twofold. Firstly, a robust ammonia coverage ratio observer was designed for estimating the ammonia coverage ratio reference for catalysts with different aging levels. An ammonia storage capacity observer was developed for estimating the actual ammonia storage capacity which can be reduced due to catalyst aging. An adaptive ammonia coverage ratio reference design was then developed to estimate the desired ammonia coverage ratio ranges at each instantaneous engine operating point for both single-cell and two-cell SCR systems at different aging levels based on a singular perturbation method. Secondly, to ensure the estimated ammonia coverage ratio falls in the desired ranges for most of engine operating conditions, robust nonlinear model predictive control (NMPC) algorithms were designed for both single-cell and two-cell SCR systems. Experimental data over US06 cycle were collected from a Diesel engine and aftertreatment system platform for controller verification. Simulation results under US06 test cycle demonstrate that the proposed NMPC algorithms were capable of consistently achieving high NO_x conversion efficiency (>95.6%) and constrained tailpipe ammonia slip (<10 ppm on average and <12 ppm on the peak) for both fresh catalyst and aged catalyst with 30% loss of ammonia storage capacity.

1. Introduction

Diesel-engine-powered ground vehicles have become more and more popular in the past decade due to their high engine efficiencies resulting from high compression ratios, lean-burn combustion, as well as the emergence of new technologies in the past decade such as low-temperature combustion (LTC), premixed charge compression ignition (PCCI), and homogeneous charge compression ignition (HCCI) [1–3]. Meanwhile, Diesel engines are commonly known for the tradeoff between engine-out NO_x emissions and particulate matter (PM) emissions, both of which have significant adverse effects on the public health and environment. Thus, Diesel engine emissions standards have been tightened to a substantial extent in the past decade [4]. However, the pursuit of lower engine emissions has become the main obstacle for modern Diesel engine development owing to the conflict between Diesel engine emissions and fuel efficiency. To address this issue, aftertreatment systems such as Diesel oxidation catalyst (DOC), Diesel particulate filter (DPF), selective catalytic reduction (SCR) system, lean NO_x trap (LNT), have emerged as indispensable components in Diesel powertrains. Particularly, urea-based SCR systems have become a standard device for removing the NO_x emissions from Diesel engine exhaust [5].

The main principles of urea-based SCR systems are described in Fig. 1. First of all, 32.5% aqueous solution, which is commonly referred to as Diesel exhaust fluid (DEF) or AdBlue, is injected into hot exhaust gas at the inlet of SCR systems. Under the hot exhaust condition, the sprayed urea solution will be decomposed into gaseous ammonia. The liberated ammonia is then adsorbed on the catalyst sites and reacts with NO_x. The ammonia coverage ratio of an SCR system is defined in Eq. (1).

$$\theta_{NH_3} = \frac{M_{NH_3}}{\Theta}, \tag{1}$$

where M_{NH_3} denotes the amount of ammonia adsorbed on catalyst sites; Θ represents the ammonia storage capacity of catalyst which

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Nomenclature

Variables and constants

C_i	molar concentration of species i, mol/m^3
F	exhaust flow rate, m^3/s
M_i	molar amount of species i, mol
R	ideal gas constant, J/mol/K
r_{ads}	adsorption rate of ammonia, 1/mol/s
r_{des}	desorption rate of ammonia, m^3/mol/s
$r_{red,f}$	reduction rate due to fast SCR reaction, 1/mol^2/s
$r_{red,s}$	reduction rate due to standard SCR reaction, 1/mol^2/s
T	temperature, K
V	volume of catalyst, m^3
θ	ammonia coverage ratio, –
$\hat{\theta}$	estimated ammonia coverage ratio, –
Θ	ammonia storage capacity, mol
$\hat{\Theta}$	estimated ammonia storage capacity, mol

Subscripts

ads	adsorption
d	desired
des	desorption
dn	downstream cell
free	free catalyst sites
in	inlet
max	maximum
min	minimum
red,f	reduction due to fast SCR reaction
red,s	reduction due to standard SCR reaction
up	upstream cell

is generally a function of catalyst temperature. According to [7], Θ decreases slowly over time as catalyst ages.

Ammonia coverage ratio is a critical index for ammonia storage quantification and SCR controls. On one hand, a high ammonia coverage ratio is preferred to achieve low tailpipe NO_x emissions but may induce high tailpipe ammonia slip. On the other hand, a low ammonia coverage ratio is favorable for maintaining low tailpipe ammonia slip but it may not provide sufficient NO_x reduction capability. The model-based ammonia coverage ratio control remains a great technical challenge. One main issue to be addressed is the design of target ammonia coverage ratio references such that high NO_x conversion efficiency and low ammonia slip can possibly be achieved. In [7–10], constant ammonia coverage ratio references were implemented for a two-cell SCR system over highly transient test cycles where the engine operating conditions experienced dynamic changes. The disadvantage of employing constant ammonia coverage ratio reference is that the emission requirements may not be satisfied at every engine operating point and only cycle-based overall emissions reduction performance can be evaluated, which makes the control strategies in these literatures less favorable in practice due to a large amount of uncertainties in the real driving cycles. For single-cell SCR systems, adaptive ammonia coverage ratio references were suggested as a function of catalyst temperature in [11–13]. A nonlinear model predictive control (NMPC)-based approach was utilized for optimizing the ammonia coverage ratio references under a test cycle for a two-cell SCR system in [14]. One concern in applying this method is the heavy computational load which prevents its real-time implementation. To address these issues, a real-time systematic approach for designing the ammonia coverage ratio references for both single-cell and two-cell SCR systems based on singular-perturbation approach using a simplified three-state (including NO concentration, NH_3 concentration, and ammonia coverage ratio) SCR model has been reported in [15]. However, this approach can be further improved in these areas in order to extend its applications. First of all, the simplified three-state SCR model may not be accurate enough to represent the actual SCR system behaviors, especially when a DOC is installed before the SCR system, since DOC has the function of converting part of NO into NO_2 and thus increase NO_2/NO_x ratio in the feedgas of SCR system. Therefore, the design of ammonia coverage ratio references based on three-state SCR model may be conservative as the benefit of fast SCR reaction to SCR performance is ignored. Secondly, the impact of catalyst aging on ammonia coverage ratio reference design has not been considered, which may prevent the designated ammonia coverage ratio references being appropriate as catalyst ages. Therefore, an ammonia coverage ratio reference that is adaptive to catalyst aging is preferred. Thirdly, it is not always possible to simultaneously achieve high NO_x conversion efficiency and low ammonia slip at every engine operating point, particularly at high flow rate and low temperatures with an aged catalyst. This issue can be addressed by coordinating active thermal management strategy with SCR control as reported in [16].

Another critical step for SCR control is the precise tracking of aforementioned ammonia coverage ratio references with high robustness against uncertainties such as the reduction of ammonia storage capacity due to catalyst aging. Since ammonia coverage ratio cannot be directly measured, it has to be accurately estimated. Although several ammonia coverage ratio observers can be found in the existing literatures, e.g. [17–19], such an observer with high robustness against the uncertainty in ammonia storage capacity and fast convergence rate is necessary but has not been reported yet. While the ammonia coverage ratio references may change fast under transient driving cycles, the ammonia coverage ratio dynamics are generally very slow due to the high ammonia storage capacity and limited control input bandwidth. Therefore, it is rather challenging to consistently place ammonia coverage ratios within the desired boundaries over transient driving cycles. Model predictive control (MPC) is an appropriate approach to address this issue as it is capable of generating optimal control input during prediction horizon while satisfying the system constraints. The

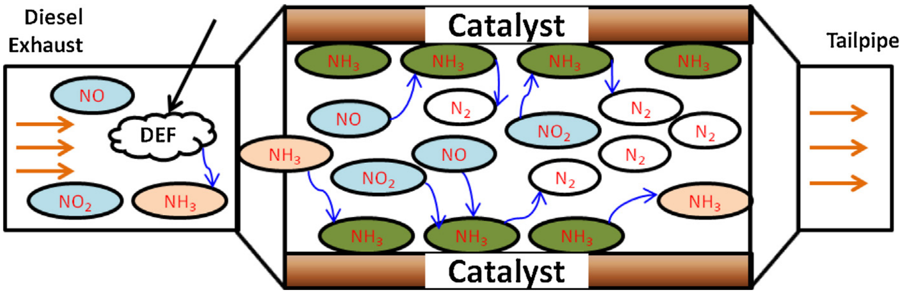

Fig. 1. Main principles of urea-based SCR system.