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Model-based optimal boundary control of selective catalytic reduction in diesel-powered vehicles

A. Aksikas [a], I. Aksikas [b,*], R.E. Hayes [a], J.F. Forbes [a]

[a] Department of Chemical and Materials Engineering, University of Alberta, Canada
[b] Department of Mathematics, Statistics and Physics, Qatar University, Doha, Qatar

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ABSTRACT

This paper is devoted to design a model-based boundary optimal controller for selective catalytic reduction system. The mathematical model consists of coupled parabolic-hyperbolic PDEs with an ODE. The main objective is to manipulate the ammonia gas at the inlet of the SCR in order to reduce the amount of NO_x and ammonia slip as much as possible. The augmented infinite-dimensional state space representation has been used in order to solve the corresponding linear-quadratic control problem. The dynamical properties of both the linearized system and its augmented version have been studied. Under some technical conditions, it has been shown that the augmented system generates an exponentially stabilizable and detectable C_0-semigroups. The linear-quadratic control problem has been solved for the augmented system. A decoupling technique has been implemented to decouple and solve the corresponding Riccati equation. An algorithm has been developed to describe the steps of solving the Riccati equation. Numerical simulations for the closed-loop system have been implemented to show the controller performances.

1. Introduction

Diesel engines are one of the most extensively used types of engines in industrial equipments and commercial vehicles especially in heavy duty ones like trains, buses, trucks and ships. This fact is due to its durability, low cost and also because of the safety of the diesel fuel since it is less volatile and its vapour less explosive [1]. In diesel engines, internal combustion rises the temperature and pressure by air compression. Then, due to this fact, the fuel-air mixture is spontaneously ignited, which in turn move pistons, transforming chemical energy into mechanical energy. However, diesel engines have many disadvantages especially environmental ones. The pollution is one of the major drawbacks of diesel engines especially the emissions of NO_x which is harmful gas and hazardous to the health [1]. To deal with this serious problem many approaches have been done in various aspects such as improvement of the fuel quality, diesel oxidation catalysts (DOC), diesel particulate filters (DPF) and also exhaust gas recirculation (EGR) to control the oxides nitrogen (NO_x) and the engine efficiency. These techniques are called after-treatment techniques. Another important technique used to reduce NO_x emissions is the selective catalytic reduction (SCR) technology, which is one of the most cost-effective technologies for this task. SCR can convert NO_x into N_2, H_2O and a small amount of carbon dioxide (CO_2) [2]. This is done by injecting the ammonia to a stream and is absorbed onto a catalyst. Nevertheless, the SCR is not a perfect method since there are some technological drawbacks such as high back pressure of pipes and space requirement, in addition to the produced ammonia slip that represents the ammonia passed through the SCR unreacted. However, when comparing to its advantages, the SCR technique is one of the most promising technologies which guarantees the reduction of toxic emissions and saves a large amount of fuel [3,4].

It has been shown that the SCR technology can reduce up to 90% percent of NO_x, but this is not the case for many reasons that affect the SCR performances such as disturbances and the continuous fluctuation related to the engine speed. Good control performance is achieved if the tailpipe concentration of NO_x is less than 50 ppm, and the ammonia slip is less than 20 ppm. The main objective of this paper is find the optimal amount of ammonia that should be injected into the SCR in order to reduce NO_x and also reduce the ammonia slip as much as possible. Unfortunately, few studies have been done to perform this task especially that the SCR model is a complex system that best described by mean of partial differential equations (PDEs). Moreover, the fact that the SCR carries out two phases (gas and solid), such that the convective mechanism is dominant in the gas phase while the diffusion mechanism is dominant in

* Corresponding author.
E-mail address: aksikas@qu.edu.qa (I. Aksikas).

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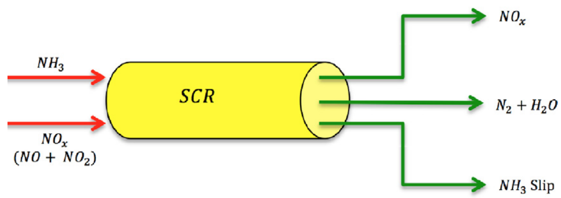

Fig. 1. SCR diagram.

the solid phase, leads to coupled system of parabolic and hyperbolic PDEs in addition to an extra ODE that describes the concentrations in the solid phase. Here, to deal with this complex system, the infinite-dimensional state-space representation is used. This representation has a main advantage of keeping the distributed nature of the system [5–7]. On the other hand and since the ammonia is injected at the inlet of the SCR, it is more appropriate to represent the process as a boundary control system.

[8] proposes a control strategy for the SCR system by using a NO_x sensor in a feedback loop. The latter uses a model obtained by mass balances for two species with three states, namely, NH_3 and NO_x in gas phase as well as adsorbed NH_3. This model neglects the energy balances equations and also neglects the distributed nature of the SCR system. On the other hand, model predictive controller has been designed for the SCR model in [9] by using the method of characteristics combined with the orthogonal decomposition method. The main drawback of this approach is that combination of the two methods leads to a reduced discrete ODE model. The number of spatial points affects the accuracy of the projection of states arise from the hyperbolic PDEs, as a result the performance of the MPC controller is affected. Here, linear quadratic control technique is used to reach the main objective and a state-feedback controller is designed on the basis of the full distributed parameter system by using infinite-dimensional state space representation. The main advantage is that the optimal input is expressed as a state feedback that guarantees the exponential stability of the closed-loop system [5,10]. The LQ-control technique has been used for both hyperbolic PDEs [11–13] and parabolic PDEs ([14–16]), including boundary control problems. Here the objective is to solve the LQ-boundary control problem for the SCR model through the corresponding Riccati operator equation.

The paper is organized as follows. Section 2 presents a brief description of the SCR process together with its dynamical models, including the full non-linear coupled parabolic-hyperbolic PDEs model, its linear version and the augmented state-space model. In Section 3, dynamical properties of the linear model and its augmented version, have been analyzed. Section 4 is devoted to solve the LQ-boundary control problem. An algorithm has been presented to solve the corresponding Riccati equation. In Section 5, Numerical simulations have been performed to show the controller performances.

2. Process description and modelling

A typical process diagram of the SCR is shown in Fig. 1.

2.1. Reaction mechanism

In order to reduce the amount of NO_x, the gaseous ammonia NH_3 is used. Indeed, it is injected through a nozzle forming an aqueous urea solution. Gaseous ammonia is formed from urea decomposition [17] through the following steps:

$$H_4N_2CO \longrightarrow NH_3 + HNCO \tag{1}$$

$$HNCO + H_2O \longrightarrow NH_3 + CO_2 \tag{2}$$

Using the formed NH_3, the nitrogen oxides emitted by the engine are reduced and converted to harmless products (nitrogen and water) over an SCR catalyst. The chemical reactions are [17]:

$$4NH_3 + 2NO + 2NO_2 \longrightarrow 4N_2 + 6H_2O \tag{3}$$

$$4NH_3 + 4NO + O_2 \longrightarrow N_2 + 6H_2O \tag{4}$$

$$8NH_3 + 6NO_2 \longrightarrow 7N_2 + 12H_2O \tag{5}$$

The most desirable pathway is the fast-SCR reaction (3), which is considerably faster than the SCR reactions (4) and (5). For high temperatures, maximum achievable NO_x conversion can be limited due to ammonia oxidation. The reaction mechanisms are [17].

$$4NH_3 + 3O_2 \longrightarrow 2N_2 + 6H_2O \tag{6}$$

$$NH_3 + 5O_2 \longrightarrow 4NO + 6H_2O \tag{7}$$

The formation of N_2O is neglected here since it is formed in smaller amount.

2.2. The complete SCR PDEs-ODEs model

The SCR catalytic converter consists of a ceramic monolith with a high amount of miniature parallel square channels. It is assumed that all channels have uniform inlet conditions so they are all identical. The SCR model can be best described by using mass and energy balance equations for both bulk and surface phases.

The mass balances of the components in the flowing gas are shown in Eq. (8), which consists of a set of hyperbolic PDEs.

$$\frac{\partial c_j^g}{\partial t} = -v\frac{\partial c_j^g}{\partial \xi} + \frac{k_m^j a}{\epsilon}(c_j^s - c_j^g), \quad j = NO, NO_2, NH_3, O_2 \tag{8}$$

The mass balances of the components in the washcoat are shown in Eq (9).

$$(1-\epsilon)\frac{\partial c_j^s}{\partial t} = k_m^j a(c_j^g - c_j^s) \pm G\sum_{k=1}^{5}\sigma_k R_k, \quad j = \mathrm{NO}, \mathrm{NO_2}, \mathrm{NH_3}, O_2 \tag{9}$$

The ammonia intermediate species surface coverage equation is given by

$$\frac{d\Omega_{\mathrm{NH_3}}}{dt} = \frac{a}{\Omega_{\mathrm{NH_3}}^{cap}}(R_{ad} - R_{des} - R_4) \tag{10}$$

The total enthalpy balance of the flowing gas is shown in Eq. (11), which also consists of a set hyperbolic PDEs.

$$\frac{\partial T^g}{\partial t} = -v\frac{\partial T^g}{\partial \xi} + \frac{h_m a}{\rho^g cp^g \epsilon}(T^s - T^g) \tag{11}$$

The enthalpy balance of the solid phase is shown in Eq. (12), which consist of one parabolic PDE.

$$\frac{\partial T^s}{\partial t} = \frac{\lambda^s}{\rho^s cp^s}\frac{\partial^2 T^s}{\partial \xi^2} - \frac{h_m a}{\rho^s cp^s(1-\epsilon)}(T^s - T^g) - \frac{h_{ext}a_{ext}}{\rho^s cp^s(1-\epsilon)}(T^s - T^{ext}) - \frac{a}{\rho^s cp^s(1-\epsilon)}\sum_{j=1}^{5}\Delta H_j R_j \tag{12}$$

All the variables and symbols used in Eqs. (8)-(12), together with the reaction rates are given in Appendix A.

2.3. SCR state-space model

The mathematical PDE model consists of a parabolic PDE coupled with a set of hyperbolic PDEs and an ODE. By using the