

Model Based Control of SCR Dosing and OBD Strategies with Feedback from NH_3 Sensors

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ABSTRACT

This paper presents a model-based control system for SCR urea dosing employing an embedded real-time SCR chemistry model and a NH_3 sensor. The control algorithm consists of a number of control features designed to enhance ammonia storage control and closed-loop compensation using the mid-brick NH_3 sensor. An adaptive control algorithm is developed to demonstrate robustness of the feedback control system to compensate for catalyst aging, urea injection malfunction, or dosing fluid concentration variation. Simulation and engine dynamometer testing following ESC and FTP emission cycles are used to demonstrate the advantages of this control approach for meeting both NO_x emission requirements and NH_3 slip targets. Furthermore this paper demonstrates potential of a NH_3 sensor for on-board diagnostics. Additionally the feasibility of implementing model based algorithms in a 32-bit floating-point environment with an automotive controller is examined.

INTRODUCTION

Selective catalytic reduction (SCR) of NO_x with aqueous urea has been proven to be a viable solution for meeting future diesel NO_x emissions standards around the world [1]. Control of the urea dosing rate, prediction of the water evaporation, urea thermohydrolysis, and potential pooling and deposit formation of urea remain the greatest challenges for assuring that NO_x reduction to US 2010 levels of 0.27 (g/kWh). Dosing control trade-off seeks to minimize NO_x while maintaining non-regulated NH_3 slip to acceptable levels of 10 ppm average and < 30 ppm peak.

Further challenge for SCR dosing systems is the need to meet the emission regulations over their in-use lifetime. Dosing errors caused by urea injector malfunction or variations in the fluid concentration pose a risk for in-use compliance. In addition, another risk factor involves degradation of both the SCR catalyst and the upstream oxidation catalyst due to thermal and chemical aging after exposure to the exhaust. Thus for real-world applications, the SCR control algorithm must provide system compensation for deterioration over its operational life. Increasingly control systems based on open-loop models and table lookup methods are not adequate to address the above mentioned challenges [2]. For this reason a closed loop urea dosing system for SCR provides an advantage for in-use compliance and for ensuring robustness of the system against aging effects and other system disturbances [2-5].

It has been suggested and validated in a simulation environment that model-based ammonia storage control combined with closed-loop NH_3 slip control provides superior performance and robustness to SCR system variations [2]. With the advent of the automotive ammonia sensor technology [6], such a control scheme can be verified on an engine dynamometer using a production feasible ammonia sensor. The subsequent study [7] indeed confirmed that the closed-loop control using NH_3 sensing feedback offers many advantages over open loop control and NO_x sensor-based closed-loop control during European Steady-State Cycle (ESC), European Transient Cycle (ETC), and Federal Test Procedure (FTP) emission cycle testing. It is noteworthy that the closed-loop control based on the NO_x sensor feedback is accurate only when driving cycles contain

extensive steady-state conditions because of its ammonia cross sensitivity issue and is therefore limited in its application [2, 7].

In the previous work [8], model-based ammonia storage control coupled with the feedback from a mid-brick ammonia sensor was explored. The ammonia sensor located at the mid-brick position of the SCR catalyst provides a quicker time response and greater sensitivity to NH_3 dosing deviation from the target because of reduced NH_3 storage capacity of the front catalyst. Combining quicker dosing response with the ammonia storage capacity of the rear catalyst helps to control ammonia slip.

The present study continues to evaluate NH_3 sensor based closed-loop control algorithm development to achieve in-use system robustness and improved transient response. ESC and FTP emission cycles were utilized to demonstrate the effectiveness of the control algorithm. In addition, on-board diagnosis (OBD) strategies with an ammonia sensor have also been explored. Finally embedding the real-time SCR chemistry model into an automotive controller has been investigated.

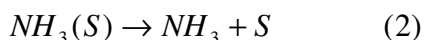
SCR CHEMISTRY MODEL

SCR 1D MODEL DESCRIPTION AND ITS CHEMISTRY

The previous paper [8] described that a one-dimensional model is a good approximation of a modern SCR catalyst, which consists of a honeycomb cordierite monolith substrate containing many small square channels. The basic governing equations are Navier-Stokes equations and the conservation of energy and species equations. For simplicity, only gas transfer and mass transport equations [8] were considered. In addition, mass transport of ammonia adsorption, desorption, and reactions are treated separately [8].

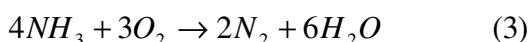
The chemical reactions for a SCR system can be very complex [9-12]. Various N_2O formation pathways [10-11], though important for an improved understanding of complex SCR chemistry, are omitted for the calibration simplicity of this model. This work considers the following main reactions.

Ammonia adsorption and desorption

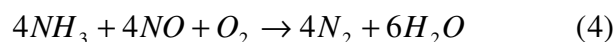


where S denotes a surface site for NH_3 storage

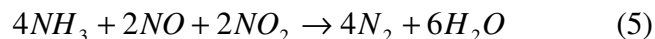
Ammonia oxidation



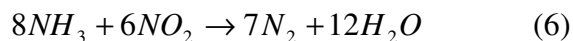
Standard SCR reaction



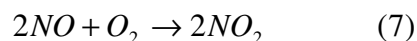
Fast SCR reaction



NO_2 SCR reaction



In addition the NO oxidation reaction is also included.



A global reaction scheme was employed for rate equations of the above individual reactions, as used widely by a majority of researchers in the field [13-19]. The transient kinetic rate expressions for the above chemical reactions were described in detail previously [8].

MODEL PARAMETER CALIBRATION

The kinetic rate equations described in the previous paper [8] contain a total of 19 global kinetic parameters that need to be calibrated for particular catalyst formulations using experimental data in order to simulate proper catalysis. The methodology for model parameter calibration using a gas bench system has been documented in detail [8]. The methodology employs a series of staged experiments which decouple the individual chemical reactions. Ammonia adsorption, desorption, and oxidation reactions, for example, can be separated from the remaining SCR reactions so that a clean calibration of the model parameters associated with the specific ammonia chemistry can be conducted without interference from NH_3 reactions to NO_x . In addition, the parameters in the standard SCR can be separated from the fast SCR and the NO_2 -SCR reactions by manipulating the composition of the input feed. Each subsequent calibration of new parameters utilizes previously calibrated parameters as the kinetics for the SCR chemistry becomes progressively more complex.

For consistency in this study, the same family of the Cu zeolite catalysts as employed previously [8] was chosen for the SCR control algorithm and OBD development. Considering possible variation in active catalytic materials and their loading inside the catalyst as well as difference in aging history from the previous catalyst, a global fit of all previously calibrated model parameters to the new catalyst using a parameter optimization software tool was performed.

The following describes the procedure for model parameter fitting. The catalyst was set up in a certain exhaust system configuration (described in the entire Dynamometer Setup section) and a custom schedule

was run. The experimental data recorded were imported to the optimization software for model parameter fitting. The SCR model input data include exhaust flow rate, the temperature, pressure, NO, NO₂, O₂ before the SCR catalyst, and NH₃ dosing quantity. During the parameter fitting procedure, the model output data (NO, NO₂, and NH₃) were compared to experimentally recorded post-SCR NO, NO₂ and NH₃ signals at each model iteration. The iterations were stopped when all model parameter converged.

SCR 1D MODEL VALIDATION

Figure 1 shows a second-by-second data comparison between model predictions and post SCR NO, NO₂, NO_x concentrations obtained in an ESC. The model predictions agree with the experiments using the fitted model parameters.

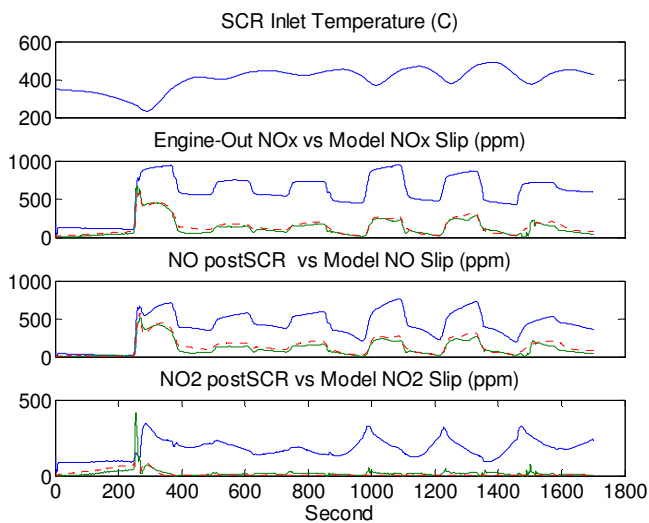


Figure 1. Pre-SCR and Post-SCR NO_x, NO, and NO₂ concentrations during an ESC emission test cycle. The dashed lines are from model simulations

ENGINE DYNAMOMETER TESTING

OBJECTIVE OF TESTING

The previous paper [8] described a two-phase approach consisting of anhydrous ammonia dosing and aqueous urea dosing to tackle SCR dosing control issues. In the first phase, a mass flow controller was utilized to dose anhydrous ammonia from a gas cylinder (99.99%, anhydrous NH₃). Gaseous NH₃ dosing provides a platform for control algorithm development and emission bench setup verification without complications associated with vaporization of aqueous urea, subsequent thermohydrolysis, urea pooling, and deposition on the upstream exhaust pipe wall. Following the first phase, a urea dosing system replaced the mass flow controller. The urea injection control system manages aqueous urea dosing.

This study employed gaseous NH₃ dosing for further algorithm and on-board diagnosis (OBD) development with feedback from the NH₃ sensor because of the above mentioned reason. The following section describes engine, exhaust system, and engine dynamometer setup.

TEST CELL SETUP

Engine and Dynamometer

A 6.6-liter, 8-cylinder turbocharged diesel engine (DuraMax) was coupled to a General Electric dynamometer load for testing. The dynamometer control is orchestrated by an AVL PUMA control system located in a separate room for safe operation.

Emission Bench Setup

Dual emission benches consisting of a number of standard emission analyzers were utilized for monitoring and recording NO, NO_x, O₂, CO, CO₂, and HC species from exhaust. Multiple sample ports located strategically along the exhaust pipe allow sampling of the exhaust before and after SCR converter (see details in the next section). The bench analyzers were calibrated on a daily basis using calibration gases. NO_x analyzers were calibrated every 4 hours during testing. A diode laser gas analyzer (LDS, Siemens) was attached to the back of the exhaust system for ammonia slip measurement. In addition, a Fourier Transform Infrared (FTIR) bench analyzer (MKS Instruments) was used for further verification of gas concentration measurement accuracy.

Exhaust System Configuration

The diesel engine exhaust is routed through the following path, as shown also in Figure 2.

1. Oxidation catalyst (DOC)
2. Sample ports: NO, NO_x, other exhaust species, temperature, and pressure measurement
3. Diesel particulate filter (DPF)
4. Sample ports: NO, NO_x, other exhaust species, NO_x sensor, temperature, pressure, and NH₃ injection
5. Mixer
6. SCR catalysts
7. Sample ports: NO, NO_x, other exhaust species, NO_x sensor, temperature, pressure, FTIR
8. LDS: ammonia slip measurement

This exhaust system setup allows the injection of anhydrous NH₃ or urea with reasonably uniform distribution along the axial direction. A separate study found that the uniformity of NH₃ gas concentration distribution behind the SCR catalyst is about 95% using this exhaust system setup.

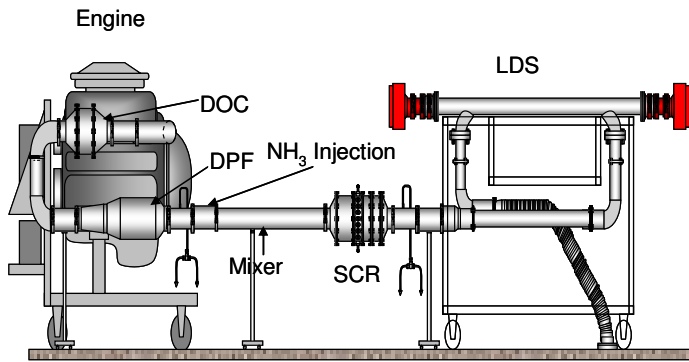


Figure 2. Exhaust system configuration consisting of DOC, DPF and SCR catalysts.

SCR Catalyst

A copper zeolite catalyst is used for testing. It consists of 3 catalyst bricks canned separately and joined either back-to-back with flanges or with a spacer ring. The spacer ring allows the installation of sample ports and ammonia sensors between catalyst bricks. This flexibility provides the opportunity to do mid-brick sensing feedback control.

Two of the catalyst bricks are 3" long and 9 1/2" in diameter. The third brick is 6" long with the same diameter of 9 1/2". Total volume of 3 catalysts is about 13.94 liters. The cell density of these bricks is 300 cells per square inch and their cordierite substrate is about 5 thousandth inch (1.27×10^{-4} m) thick.

CONTROL ALGORITHM DEVELOPMENT

CONTROL SCHEME OVERVIEW

Control of anhydrous NH_3 dosing is achieved using a high throughput development controller for control algorithm and OBD development. Figure 3 illustrates signal flow mechanization showing SCR model based control, as also described in a previous paper [8]

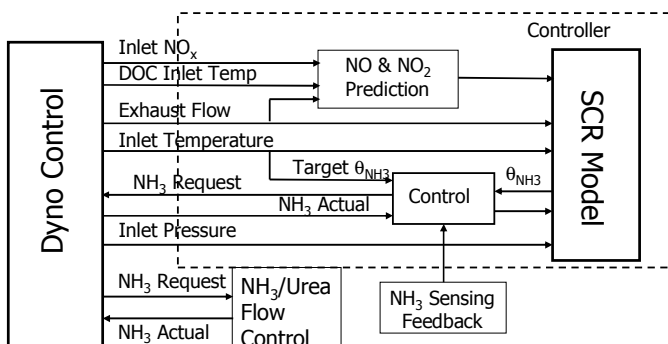


Figure 3. Signal flow mechanization showing SCR model based control

The SCR model embedded in the controller has a full access to all signals (as shown Figure 3) in real time and

calculates, among other model output signals, the amount of ammonia stored on the catalyst at a frequency of 10 Hz. The mass flow controller provides ammonia flow control. The actual flow feedback (rather than commanded NH_3 flow rate) is used by the model for computation to ensure the accurate tracking of ammonia dosing.

Figure 4 provides an overview of main features of the control algorithm.

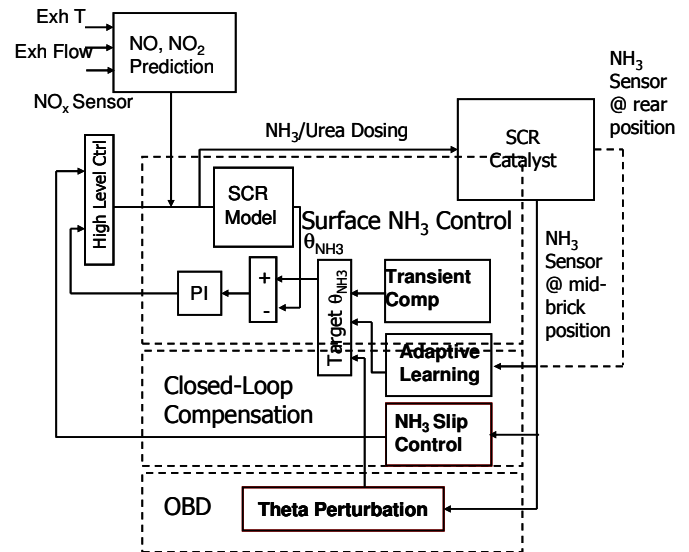


Figure 4. SCR control scheme schematic

The algorithm consists of a number of control features designed to enhance the ammonia storage control scheme and the closed loop compensation scheme. The closed loop compensation relies on NH_3 sensing feedback to achieve robustness of the control under real-world driving conditions. The following sections describe each of these control features working together to achieve maximum NO_x conversion while maintaining acceptable NH_3 slip under various driving conditions.

AMMONIA STORAGE CONTROL

As mentioned in the previous section, the algorithm utilizes an embedded SCR chemistry model to compute ammonia surface coverage (θ_{NH_3}) in real time. Real-time input signals are used to compute θ_{NH_3} . This surface coverage is then compared to target θ_{NH_3} . If a difference arises, a PI (proportion-integration) control algorithm will adjust the NH_3 dosing rate to reduce errors between computed and target θ_{NH_3} (close loop on theta).

The target θ_{NH_3} , which is a function of SCR catalyst temperature, is often set up based on the following considerations: (1) maximum possible NO_x conversion with acceptable NH_3 slip (30 ppm peak, 10 ppm average) for a given emission test cycle, and (2) limits set on ammonia storage coverage at low temperatures to prevent potential high NH_3 slip upon sudden temperature ramp up in off-cycle tests. It was found that in the ammonia storage control mode, different emission cycles