ABSTRACT

To meet 2010 emission targets, optimal SCR system performance is required. In addition, attention has to be paid to in-use compliance requirements. Closed-loop control seems an attractive option to meet the formulated goals. This study deals with the potential and limitations of closed-loop SCR control.

High NO\textsubscript{x} conversion in combination with acceptable NH\textsubscript{3} slip can be realized with an open-loop control strategy. However, closed-loop control is needed to make the SCR system robust for urea dosage inaccuracy, catalyst ageing and NO\textsubscript{x} engine-out variations. Then, the system meets conformity of production and in-use compliance norms.

To demonstrate the potential of closed-loop SCR control, a NO\textsubscript{x} sensor based control strategy with cross-sensitivity compensation is compared with an adaptive surface coverage/NH\textsubscript{3} slip control strategy and an open-loop strategy. The adaptive surface coverage/NH\textsubscript{3} slip control strategy shows best performance over simulated ESC and ETC cycles.

SCR catalyst dynamics, time delay in the urea injection and maximum NH\textsubscript{3} slip targets limit the performance of closed-loop SCR control. If new reagent dosage systems and future catalyst technology are able to relieve these limitations, closed-loop control has the potential to reduce the calibration effort and to improve the transient control performance.

INTRODUCTION

Urea SCR technology is widely accepted to meet Euro-4 emission targets for heavy-duty diesel applications. With the realization of the urea infrastructure in Europe, this technology becomes an attractive alternative for light-duty diesel applications. Moreover, urea SCR is considered as a promising technology to meet US2010 emission standards. A summary of the proposed European and US heavy-duty emission targets is given in Table 1.

<table>
<thead>
<tr>
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</thead>
<tbody>
<tr>
<td>NO\textsubscript{x} (g/kWh)</td>
<td>3.5</td>
<td>3.5</td>
<td>2.0</td>
</tr>
<tr>
<td>PM (g/kWh)</td>
<td>0.02</td>
<td>0.03</td>
<td>0.02</td>
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<tr>
<td>CO (g/kWh)</td>
<td>1.5</td>
<td>4.0</td>
<td>1.5</td>
</tr>
<tr>
<td>HC (g/kWh)</td>
<td>0.46</td>
<td>0.55</td>
<td>0.46</td>
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</table>

To meet (post-)2010 emission targets, the main challenges for urea SCR systems are:

- Maximal NO\textsubscript{x} conversion Compared to current Euro-4 levels, tailpipe NO\textsubscript{x} emissions have to be further reduced by 90% to meet 2010 targets, see Table 1. Depending on the engine-out NO\textsubscript{x} calibration, the desired NO\textsubscript{x} conversion is in the order of 70-80% for Euro-5 limits and 80-90% for US2010 limits. By optimizing the NO\textsubscript{x} conversion, safety margins associated with ageing issues and

\footnote{NMHC}
climate effects have to be reduced and the transient performance becomes important. Then, the risk of NH$_3$ slip increases; although NH$_3$ emission is not regulated, a limit of 10 ppm average NH$_3$ and 25 ppm peak NH$_3$ is often applied, see e.g., [1].

- **Enhanced low-temperature performance**
  Currently applied SCR catalysts are characterized by reduced NO$_x$ conversion for low temperatures. To optimize the NO$_x$ conversion over an FTP test cycle, performance has to be increased, especially for the relatively cold part of the cycle. Low-temperature performance is also an issue in light-duty applications.

- **Meet in-use compliance requirements**
  Besides emission targets for specified test cycles, future legislation for heavy-duty application will also include limits on performance degradation in the field. This introduces the need for SCR systems that are more robust for system variations.

As a result, optimal SCR system performance has to be realized to meet future emission legislation. This requires high NO$_x$ conversion, NH$_3$ slip suppression and improved control quality. Open-loop SCR control strategies are essentially able to achieve optimal performance over a test cycle, but this requires a considerable calibration effort. Closed-loop SCR control can relieve this calibration effort and improve dynamic control quality. More important, it offers robustness for system variations. This is essential to meet in-use compliance and conformity of production (COP) requirements.

This paper discusses the potential and limitations of closed-loop SCR control to optimize the SCR system performance. First, an overview of the current status of closed-loop SCR control is presented. From simulations with two control strategies, the achievable performance over an ESC and ETC test cycle is demonstrated. Finally, possible developments are discussed which will further improve the closed-loop SCR performance.

**SCR SYSTEM PERFORMANCE LIMITATIONS**

Figure 1 shows a typical lay-out of an engine equipped with a urea SCR system. In this system, three subsystems can be distinguished: NH$_3$ formation, catalyst, and control system. In this section, the subsystems are discussed in more detail. Focus is on performance limiting aspects.

**NH$_3$ FORMATION**

To form the required reducing agent for NO$_x$ reduction in the SCR catalyst, an aqueous urea solution (AdBlue) is injected through a nozzle, such that it is atomized in the exhaust pipe. The following steps can be distinguished in the NH$_3$ formation process [2]. Evaporation of water from the injected droplets ($T \geq 100 \, ^\circ C$). As urea starts melting at 133 $^\circ C$, it stays solid in this stage. Subsequently, the resulting urea ($H_2N-CO-NH_2$) will be decomposed in two steps:

\[
H_2N-CO-NH_2 \rightarrow NH_3 + HNCO \quad (1)
\]
\[
HNCO + H_2O \rightarrow NH_3 + CO_2 \quad (2)
\]

Thermal decomposition (1) can take place upstream of the SCR catalyst. However, the amount of formed NH$_3$ depends on temperature and space velocity. This is illustrated in [3].

From measurements in a flow reactor, it is concluded that the contribution of the hydrolysis (2) to NH$_3$ formation upstream of the SCR catalyst is negligible (Figure 2). As a result, maximal 50% of NH$_3$ is available at the SCR catalyst inlet. The hydrolysis needs to be catalyzed; this reaction occurs inside the SCR catalyst.

For optimal performance, it is important that the injected urea is well distributed over the pipe diameter; inhomogeneous distribution can lead to reduced NO$_x$ conversion and increased NH$_3$ slip. A mixing device can be applied to improve the distribution.

Possible ways to increase the formed NH$_3$ upstream of the SCR catalyst are: i) application of a hydrolysis catalyst [4]; ii) (off-line) formation of gaseous NH$_3$; iii) thermal management measures to increase the exhaust temperature.

![Figure 1: Automotive urea SCR system lay-out](image-url)
Using the formed NH₃, the nitrogen oxides (NOₓ) emitted by the engine are reduced over an SCR catalyst according to the following reaction mechanisms:

\[ 4\text{NH}_3 + 4\text{NO} + \text{O}_2 \rightarrow 4\text{N}_2 + 6\text{H}_2\text{O} \]  (3)
\[ 4\text{NH}_3 + 2\text{NO} + 2\text{NO}_2 \rightarrow 4\text{N}_2 + 6\text{H}_2\text{O} \]  (4)
\[ 4\text{NH}_3 + 2\text{NO}_2 + \text{O}_2 \rightarrow 3\text{N}_2 + 6\text{H}_2\text{O} \]  (5)

The most desired pathway is the “fast-SCR” reaction (4), which is considerably faster than the “standard SCR” reaction (3) and reaction (5). However, this path requires an NO:NO₂ ratio of 1:1. As the engine out NO:NO₂ ratio is 9:1, a pre-oxidation catalyst is applied. At temperatures down to 100 °C, NOₓ conversion can be increased up to 70% [5]. In that case, NH₃ formation is an issue when AdBlue is used as reagent.

NOₓ conversion depends on exhaust gas temperature and space velocity, see e.g. [1]. For low temperature applications, NOₓ conversion can be enhanced by measures that increase the exhaust gas temperature; e.g., throttling, post-injection in combination with an oxidation catalyst or variable valve timing.

Achievable NOₓ conversion also relies on available NH₃. For high temperatures (T > 450 °C), maximal achievable steady state NOₓ conversion is mainly constrained due to NH₃ oxidation:

\[ 4\text{NH}_3 + 5\text{O}_2 \rightarrow 4\text{NO} + 6\text{H}_2\text{O} \]  (6)

Other side reactions that can play a role are the formation of ammonium nitrate (NH₄NO₃) and the formation of nitrous oxide (N₂O), at respectively temperatures below 200 °C and above 450 °C.

For a system in which the urea decomposition is not completed before the catalyst, part of the thermolysis (1) and the entire hydrolysis (2) will take place inside the SCR catalyst. By increasing the available NH₃ on the catalyst surface, system performance is enhanced and the required catalyst dimensions can be reduced [4].

CONTROL SYSTEM

The SCR control system consists of sensors that monitor the system, a controller that computes the desired actions and a urea dosage system (see Figure 1).

With the introduction of On-Board Monitoring, the application of a post-SCR catalyst NOₓ sensor is foreseen. This sensor can be applied in closed-loop control strategies. However, current available sensors are cross-sensitive for NH₃, as illustrated in [1].

Urea dosage systems can introduce a significant time delay in the system. Achievable transient performance is strongly affected by this aspect. Therefore, it will be dealt with in this study. With the introduction of airless systems this time delay is expected to be reduced significantly.

SCR control strategies will be discussed in the next section.

SCR CONTROL STRATEGIES

The main focus in SCR control system development is to realize the desired NOₓ emission over a test cycle: nominal performance. More precisely, the urea dosage is manipulated such that a desired amount of NOₓ reduction is realized. In case a tailpipe NOₓ target is made explicit, this is often called reference tracking. With the introduction of On-Board Diagnostics (OBD) regulations, controllers that make the system robust against system variations [6] gain attention. These controllers have to deal with e.g. urea injection inaccuracy, reduced NOₓ conversion due to catalyst ageing and NOₓ engine-out variations associated with varying ambient conditions. This is often referred to as disturbance rejection. Then, compliance with real-life emission targets can be demonstrated.

This section briefly describes an open-loop strategy and gives a rough overview of the status of research into closed-loop strategies. Finally, aspects that limit the applicability of closed-loop SCR control are discussed.

OPEN-LOOP SCR CONTROL

Open-loop urea dosage strategies have proven to be sufficient to meet Euro-4 and Euro-5 emission standards.
This requires about 50-60% and 70-80% NO\textsubscript{x} reduction respectively, in a typical heavy-duty application. This open-loop or feedforward control strategy generally comprises an engine-out NO\textsubscript{x} prediction functionality, a post-catalyst NO\textsubscript{x} target and a so-called NSR map (see Figure 3).

![Figure 3: Block scheme of an open-loop SCR control strategy](image)

The desired NO\textsubscript{x} reduction is calculated as the difference between engine-out emissions and the desired post-catalyst NO\textsubscript{x} concentration. Stoichiometry gives the theoretical amount of urea needed to accomplish the desired NO\textsubscript{x} reduction. This amount is limited by a catalyst temperature and space velocity dependent NSR (Nominal Stoichiometric Ratio) map, in order to prevent maximal NO\textsubscript{x} formation.

Nominal control performance of the presented open-loop strategy over a test cycle is determined by the tailpipe NO\textsubscript{x} target and NSR map calibrations. In achieving maximal NO\textsubscript{x} conversion using this open-loop strategy, it becomes increasingly difficult to find calibrations which achieve high NO\textsubscript{x} reduction in combination with low NH\textsubscript{3} slip; especially for transient conditions (including step changes in an ESC cycle). A dynamic compensation, like a functionality which compensates for NH\textsubscript{3} adsorption and desorption, can be added to the open-loop strategy to improve control performance during transients. This introduces even more calibration effort.

Note that a pre-catalyst NO\textsubscript{x} sensor can be introduced to the presented open-loop control strategy to enhance robustness in face of varying engine-out NO\textsubscript{x} emissions.

CLOSED-LOOP SCR CONTROL

Recently, closed-loop SCR control attracts considerable attention, see, e.g., [1], [3], [7], [8]. The presented control strategies mainly rely on ammonia surface coverage control and NO\textsubscript{x} sensor feedback for Vanadium catalysts. [1] deals with the limitations corresponding to the NO\textsubscript{x} sensor’s cross-sensitivity for NH\textsubscript{3}.

Control performance improvement through the application of a closed-loop SCR control strategy is not evident. Several aspects limit the success of a closed-loop SCR control strategy:

- Slow catalyst dynamics;
- NH\textsubscript{3} slip prevention;
- Time delay in the urea dosage system.

For closed-loop control strategies that use a post-catalyst NO\textsubscript{x} sensor, the sensor cross-sensitivity can limit the performance.

Catalyst dynamics

The catalyst dynamics are linked to the extent to which a varying urea injection affects the post-catalyst NO\textsubscript{x} concentrations. NH\textsubscript{3} buffering and slow reaction kinetics filter the effect of urea dosage variations on the post-catalyst NO\textsubscript{x} concentration. If the post-catalyst NO\textsubscript{x} concentrations are insensitive to the urea dosage variations, then the SCR catalyst is said to have slow dynamics. Due to this insensitivity, high performance closed-loop control has to apply a large feedback gain. This high feedback gain can potentially destabilize the SCR system and causes an aggressive actuator signal which potentially leads to NH\textsubscript{3} slip.

If the catalyst dynamics are fast, a (high gain) NO\textsubscript{x} feedback controller is able to track a tailpipe NO\textsubscript{x} reference signal regardless of engine-out NO\textsubscript{x} dynamics and open-loop calibration. In this case, the calibration effort can be greatly reduced.

Cross-sensitivity of the NO\textsubscript{x} sensor

The cross-sensitivity of the NO\textsubscript{x} sensor to NH\textsubscript{3} can also limit the closed-loop control performance. Ignoring this cross-sensitivity causes the control loop to become potentially unstable. A control strategy that copes with the NO\textsubscript{x} sensor’s cross-sensitivity has been developed and is described in the next section. It relies on perturbing the urea injection and observing its effect on the cross-sensitive sensor signal. It is only able to compensate for slowly changing phenomena during stationary conditions.

Time delay

In an SCR system with fast dynamics, the time delay of the urea dosage system limits the performance of a closed-loop SCR control. In control engineering, delays are well known to limit control performance.

The potential of NH\textsubscript{3} slip feedback control is also limited by the time delay of the urea dosing system, but it is more heavily affected by NH\textsubscript{3} storage in the SCR catalyst.
NH₃ storage

When the catalyst shows a considerable NH₃ storage capacity, the closed-loop NH₃ controller tends to load the catalyst with NH₃, while it is pursuing a certain level of NH₃ slip. The adsorbed amount of NH₃ will desorb during the next temperature increase, probably causing NH₃ slip.

Figure 4 shows the steady-state NH₃ storage as a function of temperature for two catalyst types. From this figure, it is seen that the Vanadium catalyst can store less NH₃ than the Zeolite catalyst for a given temperature. The steady-state NH₃ storage exponentially decreases with increasing temperature. At high catalyst temperatures, the NH₃ buffering is limited and adsorption and desorption mechanisms are fast. This makes closed-loop NH₃ slip control feasible for high temperatures.

For low temperatures, the NH₃ storage has to be limited to an amount that does not cause unacceptable high NH₃ slip peaks during a sudden temperature rise. At low temperatures, these levels are considerably lower than the steady-state NH₃ storage. This kind of NH₃ slip prevention can limit the NOₓ conversion at low temperatures.

Controlling the NH₃ surface coverage of an SCR catalyst provides an ideal combination of achieving maximum NOₓ conversion and preventing NH₃ slip. Furthermore, it requires less calibration effort than SCR control strategies containing NSR maps and tailpipe NOₓ target maps.

As the surface coverage of an SCR catalyst can not be measured directly, it has to be estimated. In the next section, an SCR control strategy is presented which uses an on-line storage model to estimate the NH₃ surface coverage of the SCR catalyst. Note that as no information from feedback sensors is used in the NH₃ storage estimation, surface coverage control is essentially an open-loop strategy.

Due to the requirements associated with future emission targets, the remaining part of this study focuses on maximal NOₓ conversion. In the following sections, the potential of NOₓ and NH₃ sensor based closed-loop control strategies will be studied. These strategies will be applied to a SCR system with the following characteristics:

- Nonlinearities (including non-negative actuator constraint);
- Time delay in the dosage system;
- NH₃ emission constraints;
- Cross-sensitivity of NOₓ sensor for NH₃.
The engine-out NO\textsubscript{x} prediction is based on an engine specific map of nominal NO\textsubscript{x} emissions. These steady-state values are corrected for dynamic temperature effects through first order filters.

The desorption compensation block is included to compensate for NH\textsubscript{3} desorption during temperature transients. It is based on the steady state NH\textsubscript{3} storage data presented in Figure 4. During a temperature increase a certain amount of NH\textsubscript{3} will desorb from the catalyst surface. This amount is subtracted from the urea or NH\textsubscript{3} injection amount dictated by the NSR map, in order to prevent NH\textsubscript{3} slip.

**NO\textsubscript{x} SENSOR BASED CONTROL**

The structure of the proposed NO\textsubscript{x}-sensor based controller is presented in Figure 6. The strategy modulates a block signal on the nominal urea injection, and observes the signal from the cross-sensitive NO\textsubscript{x} sensor. Urea is alternately overdosed and underdosed with respect to the average urea dosage. The chosen amplitude and period of the block signal are dependent on the SCR catalyst dynamics and operating point. The effect of the urea dosage variations have to be clearly observable in the NO\textsubscript{x} sensor signal. The urea perturbation is stopped during low temperature regimes. Under these conditions, the SCR catalyst dynamics prevent the urea injection variations to be observable in the NO\textsubscript{x} sensor signal.

If the urea injection is raised and a decreasing NO\textsubscript{x} sensor signal is recorded, then it is safe to further increase the average injection rate. In case an increased urea dosage results in an increasing sensor signal, then NH\textsubscript{3} slip is detected and the urea dosage needs to be lowered. Vice versa, a decreased urea dosage resulting in a decreased sensor signal indicates NH\textsubscript{3} slip.

For the algorithm to function properly, stationary SCR operating conditions are required; i.e., stationary NO\textsubscript{x} engine-out emissions and exhaust flow. Transient conditions make it impossible to judge whether a change in NO\textsubscript{x} sensor signal has been caused by the varying urea injection, or by variation of another quantity (e.g. engine out NO\textsubscript{x} or temperature variations). This property limits the performance of the proposed control strategy. It is only able to compensate for the effects of slowly changing phenomena like ambient conditions.

The NO\textsubscript{x} sensor based control strategy relies on the map based open-loop strategy for the nominal urea dosage. The tailpipe NO\textsubscript{x} target map is consequently calibrated for NO\textsubscript{x} levels which correspond to the steady state post-catalyst NO\textsubscript{x} concentrations which are achieved by the map based open-loop strategy.

**ADAPTIVE SURFACE COVERAGE / NH\textsubscript{3} SLIP CONTROL**

In closed-loop NH\textsubscript{3} control, maximum NO\textsubscript{x} conversion is pursued under a given NH\textsubscript{3} slip constraint. However, depending on the NH\textsubscript{3} buffering on the SCR catalyst, NH\textsubscript{3} slip feedback control is only feasible at high and increasing catalyst temperatures. Under ‘low’ or decreasing temperature conditions, an NH\textsubscript{3} slip feedback controller tends to load the SCR catalyst with NH\textsubscript{3}.

In order to prevent uncontrollable NH\textsubscript{3} slip, the NH\textsubscript{3} storage on the SCR catalyst needs to be limited. Surface coverage control limits this amount to a level that maintains a considerable NO\textsubscript{x} conversion, but prevents NH\textsubscript{3} slip in case of an increasing temperature transient. The surface coverage reference map (θ map) in Figure 7 is calibrated to prevent undesired NH\textsubscript{3} slip peaks during a severe temperature rise.

The NH\textsubscript{3} storage or surface coverage of an SCR catalyst cannot be measured directly and has to be estimated. Besides NH\textsubscript{3} adsorption/desorption mechanisms, the actual NH\textsubscript{3} storage depends on NO\textsubscript{x} conversion chemistry, NH\textsubscript{3} oxidation and possible side reactions with
NH₃. For current simulations, the same SCR model is used for surface coverage prediction and SCR catalyst simulation. A sensitivity study has pointed out that 20% discrepancy in the surface coverage prediction causes less than 2% increase of total NOₓ emissions during steady state and an ETC driving cycle. This observation suggests that a simplified, less accurate model can be used for surface coverage prediction.

The open-loop surface coverage control is combined with the closed-loop NH₃ slip control to provide robustness and adaptation capabilities. The control mode switching & adaptation block in Figure 7 adapts the θ map such that NH₃ slip feedback control mode is active during high and increasing catalyst temperatures and surface coverage control is active during low and decreasing temperatures. The developed controller is capable of adapting to changing conditions.

**SIMULATION RESULTS**

The three presented control strategies are evaluated using TNO’s simulation tool SimCat. More information on this simulation tool is presented in the appendix. The simulated SCR system contains two parallel Vanadium SCR bricks with a length of 12 inch and a diameter of 10.5 inch, making the total catalyst volume about 34 liters. In the model, complete urea decomposition is assumed upstream of the SCR catalyst. The injection system is assumed to impose a time delay of 0.5 s. Engine-out data has been gathered from a Euro-2 315 kW heavy-duty diesel engine with a swept volume of 12 liter.

The three control strategies are evaluated for maximal NOₓ conversion using ESC simulations for a nominal case, and a case in which engine-out NOₓ emissions are increased by 30%. This second case simulates the effects of climate and engine variation on engine-out NOₓ emissions [9], and serves to evaluate the robustness of the closed-loop controls. The simulated ESC emission results are presented in Table 3. Figure 8 shows the ESC simulation traces for the 30% increased engine-out NOₓ case.

As the control strategy based on NOₓ feedback is based on the map based open-loop strategy, it applies little correction and achieves comparable NOₓ and NH₃ emissions for the nominal case, as can be seen in Table 3. The adaptive surface coverage/NH₃ slip control strategy shows a NOₓ cycle result of 0.87 g/kWh and excels in avoiding NH₃ slip by limiting the surface coverage. It demonstrates a maximum slip level of 24 ppm, whereas the open-loop and NOₓ sensor based control strategies show a maximum NH₃ slip peak of about 90 ppm over the ESC cycle.

Figure 8 shows how the NOₓ sensor based control strategy and the adaptive surface coverage/NH₃ control slowly increase the reagent dosage in order to compensate for the increased engine-out emissions. The map based open-loop strategy is not able to compensate for the increased engine-out NOₓ emissions as it uses a prediction of nominal engine-out NOₓ concentrations instead of an engine-out NOₓ sensor. The post-catalyst NOₓ concentrations for the NOₓ sensor based strategy slowly converge to the nominal open-loop NOₓ levels which were calibrated through the tailpipe NOₓ target map. Adaptive surface coverage/NH₃ control again avoids excessive NH₃ slip. It increases the reference NH₃ storage and consequently the reagent injection, until it is able to control the NH₃ slip at a 10 ppm level during the relatively hot ESC modes.

The emission results for the 30% increased engine-out NOₓ case presented in Table 3 correspond to the traces in Figure 8. The cross-sensitive NOₓ feedback and adaptive surface coverage/NH₃ control strategies show an improved NOₓ conversion in comparison to the open-loop strategy, but the cycle NOₓ emissions are significantly higher than the NOₓ emissions for the nominal engine-out NOₓ case. The cycle results improve when the strategies are allowed to adapt to the 30% increased NOₓ situation before the cycle result are recorded. In this case, the NOₓ sensor based strategy accomplishes a NOₓ cycle result of 0.82 g/kWh, but shows an unacceptable high NH₃ slip peak. For the adaptive surface coverage/NH₃ slip control strategy, the NOₓ emissions over the ESC cycle drop to 1.36 g/kWh, while the average and maximum NH₃ slip are 5 ppm and 16 ppm respectively.

The map based open-loop strategy and the adaptive surface coverage/NH₃ control strategy are also compared over the ETC cycle. The ETC performance of the NOₓ sensor based feedback strategy is not considered, because this strategy is only applicable in stationary conditions. The NOₓ sensor based control strategy is not able to apply any corrections during the ETC cycle and will achieve a control performance similar to the open-loop performance.

Table 3. ESC simulation results

<table>
<thead>
<tr>
<th>Engine-out NOₓ</th>
<th>Control strategy</th>
<th>g NOₓ / kWh</th>
<th>avg. NH₃ slip (ppm)</th>
<th>max. NH₃ slip (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nominal</td>
<td>Map based open-loop</td>
<td>0.78</td>
<td>9</td>
<td>91</td>
</tr>
<tr>
<td>Cross-sensitive NOₓ feedback</td>
<td>0.83</td>
<td>8</td>
<td>89</td>
<td></td>
</tr>
<tr>
<td>Adaptive θ/NH₃ control</td>
<td>0.87</td>
<td>6</td>
<td>24</td>
<td></td>
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<tr>
<td>30% increased</td>
<td>Map based open-loop</td>
<td>2.09</td>
<td>2</td>
<td>12</td>
</tr>
<tr>
<td>Cross-sensitive NOₓ feedback</td>
<td>1.25</td>
<td>6</td>
<td>45</td>
<td></td>
</tr>
<tr>
<td>Adaptive θ/NH₃ control</td>
<td>1.63</td>
<td>3</td>
<td>15</td>
<td></td>
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</table>
Table 4 demonstrates that the adaptive surface coverage/NH\textsubscript{3} slip control strategy shows a control performance superior to the map based open-loop strategy when it comes to both NO\textsubscript{x} conversion and NH\textsubscript{3} slip prevention. For this dynamic cycle, its surface coverage control is better suited to achieve high NO\textsubscript{x} conversion than the map-based open-loop calibration strategy.

The NH\textsubscript{3} feedback mechanism allows compensation for the increased engine-out NO\textsubscript{x} emissions; the tailpipe NO\textsubscript{x} emissions have been lowered by 32\% relative to the open-loop performance in case of the 30\% increased engine-out NO\textsubscript{x} emissions.

For maximal NO\textsubscript{x} conversion, the maximum NH\textsubscript{3} slip constraint of 25 ppm seems hard to satisfy according to the presented simulation results. The open-loop map based strategy and the NO\textsubscript{x} sensor based strategy show large NH\textsubscript{3} slip peaks, especially during ESC simulations. Surface coverage control offers the best solution of preventing NH\textsubscript{3} slip peaks.

The demonstrated emission levels are not yet near the levels required by the US2010 standard: 0.27 g NO\textsubscript{x}/kWh. SCR system improvements as well as measures to decrease engine-out NO\textsubscript{x} emissions will be necessary to further lower tailpipe NO\textsubscript{x} emissions.

Table 4. ETC simulation results

<table>
<thead>
<tr>
<th>Engine-out NO\textsubscript{x}</th>
<th>Control strategy</th>
<th>g NO\textsubscript{x} / kWh</th>
<th>avg. NH\textsubscript{3} slip (ppm)</th>
<th>max. NH\textsubscript{3} slip (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nominal</td>
<td>Map based open-loop</td>
<td>2.67</td>
<td>3</td>
<td>48</td>
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<tr>
<td></td>
<td>Adaptive $\theta$/NH\textsubscript{3} control</td>
<td>1.66</td>
<td>3</td>
<td>34</td>
</tr>
<tr>
<td>30% increased</td>
<td>Map based open-loop</td>
<td>4.22</td>
<td>1</td>
<td>29</td>
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<tr>
<td></td>
<td>Adaptive $\theta$/NH\textsubscript{3} control</td>
<td>2.88</td>
<td>2</td>
<td>33</td>
</tr>
</tbody>
</table>

Table 4. ETC simulation results

The NH\textsubscript{3} feedback mechanism allows compensation for the increased engine-out NO\textsubscript{x} emissions; the tailpipe NO\textsubscript{x} emissions have been lowered by 32\% relative to the open-loop performance in case of the 30\% increased engine-out NO\textsubscript{x} emissions.

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DISCUSSION

Besides the selected control strategy, the achievable performance is strongly affected by the characteristics of the studied system. To realize optimal SCR system performance, an outlook is given on which developments are desirable from a control point of view.

Catalyst

The SCR system dynamics are dominated by the relatively slow surface coverage dynamics. As illustrated in [10], fast dynamics are favorable to reduce calibration time; in that case, an open-loop calibration is no longer required. However, it will serve as a fall-back strategy in case the feedback sensor fails.

To optimize the performance of the SCR catalyst, a pre-oxidation catalyst will be applied. This does not fundamentally change the closed-loop SCR strategy; generally speaking, low temperature NO\textsubscript{x} conversion will be enhanced.

Zeolite SCR catalysts are supposed to be applied to meet future emission targets. These catalysts are characterized by high steady-state NO\textsubscript{x} conversion and relatively high NH\textsubscript{3} storage capacity (see Figure 4), which makes the NH\textsubscript{3} slip control more challenging.

To guarantee negligible NH\textsubscript{3} slip, an NH\textsubscript{3} oxidation catalyst can be placed downstream of the SCR catalyst. To make this an attractive option for future systems, the NH\textsubscript{3} conversion and selectivity of state-of-the-art NH\textsubscript{3} oxidation catalysts has to be improved.

Urea dosage system

Due to the relatively slow catalyst dynamics, the time delay in the dosing system seems currently not the most limiting factor on performance. However, it constrains the closed-loop system dynamics. With the use of airless dosage systems, the time delay can significantly be reduced. Then, the nominal performance can be enhanced for systems with fast catalyst dynamics. This will result in less calibration effort and increased NO\textsubscript{x} conversion over a dynamic test cycle.

Sensors

With the introduction of future OBD requirements, measurement of tailpipe NO\textsubscript{x} emissions will be required. Therefore, the application of a post-SCR catalyst NO\textsubscript{x} sensor is foreseen. Its cross-sensitivity complicates the use in closed-loop SCR control strategies. In the presented study, the adaptation speed is slow and tailpipe NO\textsubscript{x} can not be reduced below a specific value (minimum of NO\textsubscript{x} + NH\textsubscript{3} concentrations added) due to the cross sensitivity characteristic of the sensor. An SCR catalyst model could help in estimating the fractions NO\textsubscript{x} and NH\textsubscript{3} in the cross-sensitive sensor signal, but this requires an accurate model.

NH\textsubscript{3} slip feedback is limited to high temperature operating conditions, whereas NO\textsubscript{x} feedback control can be applied in all operating conditions. Realization of a specified tailpipe NO\textsubscript{x} level is only possible if a model can predict this level. Furthermore, production type NH\textsubscript{3} sensors are expected not to be available within a few years. This makes NO\textsubscript{x} sensor based closed-loop SCR control solutions most promising. Especially, when new sensor technology is able to cancel the cross-sensitivity problem.

With the introduction of fast SCR system dynamics, the need for high bandwidth sensors will grow. Moreover, sensor accuracy and durability becomes more important when maximal NO\textsubscript{x} conversion is required.

Interaction with engine and DPF

Finally, it is foreseen that SCR systems will be combined with DPF systems to meet future emission targets. In case a DPF is placed upstream of the SCR system, integration aspects have to be assessed, see e.g. [11]; the DPF can influence the NO/NO\textsubscript{x} ratio upstream of the SCR catalyst and the exhaust gas temperature due to thermal inertia of the DPF or during active regeneration. In the end, the performance of the combined system of engine, DPF and SCR system is of interest. This combined system has to achieve the desired tailpipe emission with minimal fuel consumption and acceptable drivability. This requires an integrated approach: Integrated Emission Management. In that case, the engine is controlled such that the required conditions (emissions, exhaust gas temperature) are realized for the DPF and SCR system; for instance, using engine measures to increase the exhaust gas temperature during a specific period in time.

CONCLUSIONS

To meet future emission targets, SCR systems have to achieve maximal NO\textsubscript{x} conversion in combination with minimal NH\textsubscript{3} slip. In this study, the potential and limitations of closed-loop SCR systems are discussed to realize optimal performance.

From the reported results, the following can be concluded:

- Closed-loop SCR control is essential to meet in-use compliance requirements. Main benefit is that it adds adaptation capabilities and robustness for system variations. Closed-loop control is not required to enhance nominal performance over a test cycle for the current SCR systems.

- Performance of closed-loop SCR control is limited due to slow catalyst dynamics, a time delay in the urea dosage and limits on NH\textsubscript{3} emission. Large NH\textsubscript{3} buffering capacity of an SCR catalyst limits the
applicability of NH₃ slip feedback control and exposes the need for surface coverage control.

- The presented adaptive surface coverage/NH₃-slip control strategy achieved highest NOₓ conversion with minimal NH₃ slip over an ESC and ETC cycle, for the studied SCR system with time delay in urea injection. The NOₓ sensor based strategy with cross-sensitivity compensation is only able to compensate for slowly changing phenomena during stationary conditions.

- If reagent dosage systems and future sensor and catalyst technology relieve the specified limitations, closed-loop SCR control has the potential to reduce the calibration effort and to improve transient control performance.

Future work will focus on the demonstration of control strategies on an experimental set-up and on the further development of the SCR system model. Control developments also have to concentrate on the interaction of the SCR system with the engine and DPF system: Integrated Emission Management.

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APPENDIX

TNO’s SimCat is a tool for exhaust gas after treatment system modeling in MATLAB/Simulink®. With this modular tool, various SCR system configurations can be modeled. It consists of one dimensional models for urea decomposition in the exhaust pipe, pre-oxidation catalyst, SCR catalyst and an NH₃ oxidation catalyst. These models are based on first principle modeling, including mass and energy balances.

The SCR catalyst model takes exhaust flow, upstream exhaust gas temperatures and upstream concentrations of several species as its inputs. The model predicts quantities like NOx conversion, NH3 slip and temperatures as a function of the location in the catalyst and as a function of time. The modeled chemical reactions are shown in Figure 9. A description of the reactions can be found in [2] and [9].
The applied models are validated using flow reactor data and engine dynamometer data. As shown in Figure 10, the model shows good agreement with flow reactor measurements.

Figure 10. Flow reactor experiments and model fit of a Vanadium catalyst using NH₃ reagent at 250 °C and space velocity of 100,000 h⁻¹

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