Preprints of the 19th World Congress
The International Federation of Automatic Control
Cape Town, South Africa. August 24-29, 2014

SCR Ammonia Dosing Control by a Nonlinear Model Predictive Controller

Stephan Stadlbauer * **Harald Waschl** * **Luigi del Re** *

* *Institute for Design and Control of Mechatronical Systems Johannes Kepler University Linz, Austria (e-mail: stephan.stadlbauer@jku.at, harald.waschl@jku.at, luigi.delre@jku.at).*

Abstract: To deal with the demanding goals of the restricted Diesel emission legislation the focus in the application of exhaust after treatment systems to fulfill these strict requirements moves more and more to model based design, optimization and control.
Against this background a nonlinear model predictive control (MPC) for an exhaust after treatment system consisting of a DOC (Diesel oxidation catalyst), a DPF (Diesel particulate filter) and a SCR (selective catalytic reduction) is proposed. Similar to standard ammonia control schemes also in this study the dosing amount is the only adjustable input variable. But in contrast to these usually simple feed forward dosing approaches in this proposal also information about the nonlinear temperature behavior and the storage effects of the SCR - included in a nonlinear SCR model - can be considered for the ammonia control. Based on these improved knowledge of the system a nonlinear model predictive controller, also applicable for real time tests on the engine, is applied for SCR control leading to promising results in simulation.

1. INTRODUCTION

The emissions of modern Diesel engines, which are known to have various health effects are besides the drivers torque demands and low fuel consumption one of the most challenging targets for combustion and after treatment control. To comply with legal requirements (see e.g. Johnson [2013]), NO_x emission control for heavy duty Diesel engines is not feasible without additional hardware, usually consisting of a Diesel oxidation catalyst (DOC), a Diesel particulate filter (DPF) and a selective catalytic reduction (SCR) system.
While the main purpose of the DOC is the oxidation of carbon monoxide to carbon dioxide, NO to NO_2 and hydro carbons, the DPF filters the soot particles and the SCR is mainly responsible for the reduction of the NO_x emissions. Different from engine internal NO_x reduction techniques like EGR (exhaust gas recirculation) (Zheng et al. [2004]), or Lean NO_x traps (LNT) for the SCR an additional reacting agent is required to reduce the NO_x to nitrogen and water. Therefore in many of the conventionally available SCR layouts Adblue, a liquid with 32.5 % urea solution, is injected in front of the SCR to vaporize and produce the necessary ammonia for the NO_x reduction.
Whichever approach for exhaust after treatment is chosen, the demanded requirements make it necessary to investigate the arising phenomena's precisely. Therefore the proposed models have to be precise to achieve on one hand an accurate estimation and as a result of this accuracy also a precise control scheme. In literature various investigations for modeling and control of the different after treatment devices are presented. The proposed SCR models are in the range from detailed high prediction quality models suitable for system analysis (Sharifian et al. [2011]) to control oriented modeling approaches as shown in (Schär et al. [2006] and Zanardo et al. [2013]).
In Willems et al. [2007], McKinley and Alleyne [2012] and Hsieh and Wang [2009] different SCR- and an LNT control schemes are discussed. Regarding the DPF and the DOC, Jung et al. [2008] and Chatterjee et al. [2008] present modeling and experimental results, where the main focus lies on a detailed DPF model and the behavior of aged DOCs.
On contrary to these proposals in this work only the behavior of the SCR and its optimal ammonia dosing control is investigated more in detail. The additional hardware in such an exhaust after treatment system namely the DPF and the DOC, although important for other emissions like soot and CO, are not considered in this case. In principle three main mechanisms are taking place in the SCR for the NO_x reduction with ammonia.

$$4NH_3 + 4NO + O_2 \rightarrow 4N_2 + 6H_2O \quad (1)$$

$$4NH_3 + 3NO_2 \rightarrow \frac{7}{2}N_2 + 6H_2O \quad (2)$$

$$4NH_3 + 2NO + 2NO_2 \rightarrow 4N_2 + 6H_2O \quad (3)$$

As it is shown in (1), (2), (3) a separation into three different reactions and reaction speeds can be done. Whilst the reactions only with NH_3 and NO or NO_2 are relatively slow the speed increases significantly if the same amount of NO and NO_2 is available to react with NH_3. As consequence and due to the length and volume of the used SCR the fastest reaction is primarily responsible to fulfill the overall conversion requirements. If that circumstance is not considered a too high amount of ammonia at the outlet may not only caused by a too high dosing of NH_3 according to the NO_x emissions but also due to an unbalanced NO to NO_2 ratio. Apart from that the SCR possess also a ammonia storage effect which appears if a too high amount

of ammonia is injected. First this too large dosing is not detectable but after a certain time, depending on the volume of the SCR, an ammonia slip becomes observable. But with regard to the 10ppm NH_3 limit at the outlet it is too late to react and fulfill these emission requirement. Due to this storage effect it is important to create a model which covers not only the NO_x and NH_3 behaviors at the outlet but also the ammonia surface coverage which can be seen as a strong related quantity to the ammonia filling level of the SCR (see also Schär et al. [2006]). These combinations and the circumstance that all these phenomena's have highly nonlinear temperature dependencies, forces the combination of a non linear physical and a data based approach to model the SCR behavior (see also Zanardo et al. [2013]). As result of this nonlinear modeling also for control a non linear MPC strategy seems an intuitive choice.

In the early nineties the MPC was mainly used for petrochemical applications (see e.g Qin and Badgwell [2007]), where only quasi steady state conditions with high time constraints and sampling times are occurring. But nowadays with recent developments of fast tailored solvers and increased computational power, new possible fields for the application of MPC are enabled. These new applications involve tight model specifications, adaptations as consequence of operation point changes and the frequently effort in the development and implementation of efficient solutions of optimization problems especially for the NMPC (see e.g. Magni et al. [2009]).

Against this background in this work the NMPC is applied to an ammonia filling level control based on a nonlinear gray box model shown in Zanardo et al. [2013]. In order to implement a NMPC which is directly applicable for real time tests, e.g. on a test bench, the ACADO toolkit (see Ariens et al. [2010]) equipped with an efficient solution for the optimization problem in real time is used in this simulation study.

The rest of this work is structured as follows: first the system and experimental setup used for identification and validation of the SCR model is presented. Afterwards a physical SCR model with a data based extension is described and the NMPC NH_3 dosing strategy based on the SCR filling level is introduced. This is followed by the simulation results of the proposed control scheme and finally the findings of this work are summarized and concluded.

2. SCR MODEL

In order to develop the NMPC strategy, first a model for the SCR reduction mechanism is required. Subsequently in the next chapter this model is described and further details can be found in Zanardo et al. [2013].

2.1 System Setup

The required measurements to obtain data for the SCR model were carried out on a highly dynamical engine test bench at the Johannes Kepler University in Linz (see Fig. 1). The considered test candidate was a 4 cylinder 7-liter heavy duty off-road Diesel engine with a maximum torque of 1115Nm @ 1500 rpm and a maximum power of 175kW @ 2000 rpm. This engine is equipped with a common rail injection system, an external exhaust gas recirculation and a two stage turbocharger with waste gate and a SCR system.

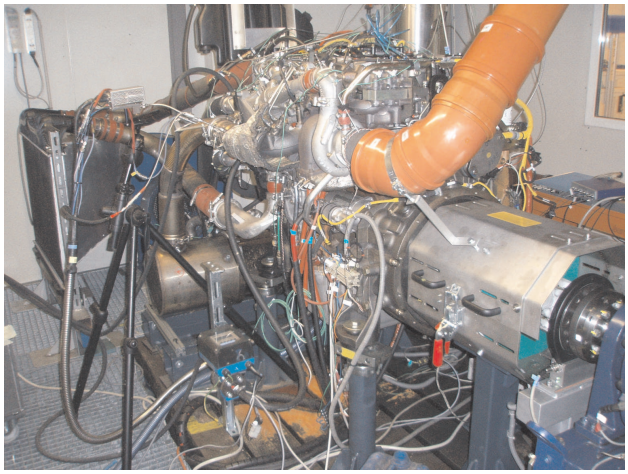

Fig. 1. Heavy duty Diesel engine setup

In order to achieve valid NO_x emissions before and after the SCR for model calibration and verification, a Horiba 6000 measuring the NO, NO_2 and NH_3 concentration is used. A general overview of the different measurement positions is shown in Fig. 2.

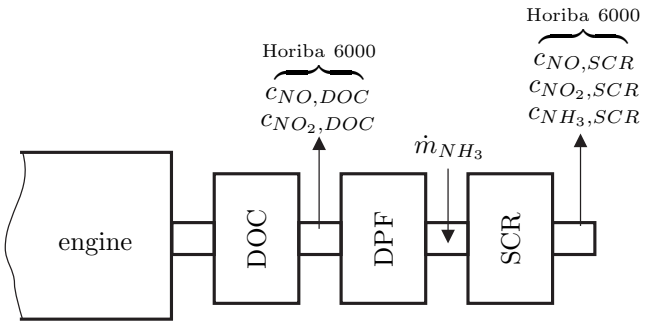

Fig. 2. Structure of the utilized exhaust after treatment system

2.2 Physical based SCR modeling

In order to include all relevant phenomena's of the NO_x reduction, but also avoid an unnecessary complex structure of the model, first some general assumptions to simplify the SCR model are made:

(1) Only adsorbed NH_3 is involved in the NO_x conversion, while NO_x reacts from the gas phase (Eley-Rideal mechanism)

$$NH_3(g) \longleftrightarrow NH_3(ads) \tag{4}$$

(2) Only the NO_x amount with equal NO to NO_2 ratio will be considered for the SCR reactions

$$4NH_3(ads) + 2NO + 2NO_2 \rightarrow 4N_2 + 6H_2O \tag{5}$$

(3) The dynamics of NH_3 adsorption/desorption on the catalyst surface is much slower than the other reactions

(4) Oxidation of adsorbed NH_3 is also considered

$$4NH_3(ads) + 3O_2 \rightarrow 2N_2 + 6H_2O \tag{6}$$

The resulting PDEs necessary to describe the behavior of the catalytic converter based on the previous assumptions are approximated by ODEs by partitioning the converter into a number of idealized SCR cells (in this investigations a SCR model consisting of 3 cells is considered). Additionally the variables of each cell are also assumed to be homogeneous.
This leads to the following three equations, in which a_0-a_6 are physical parameters see Zanardo et al. [2013]. θ_{NH3} represents the surface coverage or filling level of the catalyst limited between 0 and 1, c_{NOx} the concentration of the NO_x emissions and c_{NH3} the NH_3 level at the outlet of the SCR. T describes the temperature of the SCR, $n_{NOx,in}$ is the molar NO_x flow rate at the inlet of the SCR and m_{EG} is the exhaust mass flow.

$$c_S\dot{\Theta}_{NH3} = a_3(T)(1-\Theta_{NH3})c_{NH3} - [a_4(T)+a_5(T)c_{NOx}+a_6(T)]\Theta_{NH3} \quad (7)$$

$$c_{NOx} = \frac{a_1 n_{NOx,in}}{a_0 a_1 m_{EG} T + a_5(T)\Theta_{NH3}} \quad (8)$$

$$c_{NH3} = \frac{a_1 n_{NH3,in} + a_4(T)\Theta_{NH3}}{a_0 a_1 m_{EG} T + a_3(T)(1-\Theta_{NH3})} \quad (9)$$

To characterize the necessary parameters in a_0-a_6 various experimental tests in different engine operation points and under different dosing conditions are performed. After solving the nonlinear optimization problem (see Zanardo et al. [2013]), the obtained parameters are validated with several test cycles. The results of one of these validation experiments are shown in Fig. 3 and Fig. 4. For these as well as for all following figures the emissions are always normalized to the maximum emissions.

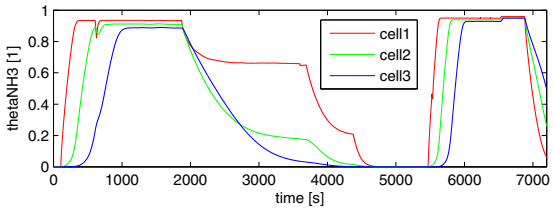

Fig. 3. Validation of the SCR surface coverage for the three proposed cells

If the figures are compared it is evident that if the filling level of each cell exceeds approximately 0.85 NH_3 slip becomes detectable at the outlet of the SCR. Therefore the filling level can be used as indicator for slip estimation which is indeed important for the SCR dosing control.
Although a good model prediction quality is achievable in validation (apart from inhibition effects see Sharifian et al. [2011]) with regard to the NMPC the model should be improved to further reduce the model plant mismatch. Hence, in addition to the physical based approach a data based extension is requested to improve the model quality.

2.3 Data based extension

The applied data based approach is based on the assumption that the error between the physical model and the measurements can be estimated by equation (10).

$$y(k) = f(\boldsymbol{u}(k-j), y(k-j), \boldsymbol{\theta}) + e(k-1) \quad (10)$$

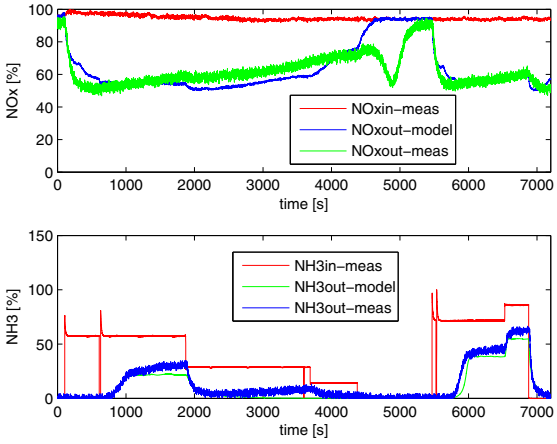

Fig. 4. Validation of the NO_x and NH_3 emissions after the SCR

$y(k)$ is the quantity to be modeled, $\boldsymbol{u}(k-j)$ is a vector of i inputs and j time shifts, $e(k-1)$ is a zero mean white noise representing measurement and modeling errors, assumed to be uncorrelated with f, $\boldsymbol{\theta} = [\theta_1, \ldots, \theta_J]^T$ is a parameter vector and J is the number of the parameters. Since these models are linear in the parameter vector $\boldsymbol{\theta}$ a standard least squares technique (Ljung [1999]) can be applied to estimate the parameter vector $\hat{\boldsymbol{\theta}}$ shown in (11).

$$\begin{aligned}\hat{\boldsymbol{\theta}} &= \arg\min_{\theta} \sum_{k=1}^{N} \left(y(k) - \boldsymbol{\varphi}^T(k)\boldsymbol{\theta}\right)^2 \\ &= \left(\frac{1}{N}\sum_{k=1}^{N}\boldsymbol{\varphi}(k)\boldsymbol{\varphi}^T(k)\right)^{-1}\frac{1}{N}\sum_{k=1}^{N}\boldsymbol{\varphi}(k)y(k) \\ &= \left(\boldsymbol{\Phi}^T\boldsymbol{\Phi}\right)^{-1}\boldsymbol{\Phi}^T\boldsymbol{Y},\end{aligned} \quad (11)$$

With respect to the considered inputs the temperature T, the exhaust mass flow m_{EG} and the concentration of the NO_x emissions cNO_x, the following estimations of the NO_x and NH_3 errors (e_{NOx} respectively e_{NH3}) are made.

$$\begin{aligned}e_{NOx}(k+1) = {} & \theta_1 e_{NOx}(k) + \theta_2 e_{NOx}(k-1) + \\ & \theta_3 e_{NOx}(k-2) + \theta_4 m_{EG}(k) + \\ & \theta_5 m_{EG}(k-1) + \theta_6 T(k) + \\ & \theta_7 T(k-1) + \theta_8 c_{NOx}(k) + \\ & \theta_9 c_{NOx}(k-1)\end{aligned} \quad (12)$$

$$\begin{aligned}e_{NH3}(k+1) = {} & \theta_{11} e_{NOx}(k) + \theta_{12} e_{NOx}(k-1) + \\ & \theta_{13} e_{NOx}(k-2) + \theta_{14} m_{EG}(k) + \\ & \theta_{15} m_{EG}(k-1) + \theta_{16} T(k) + \\ & \theta_{17} T(k-1) + \theta_{18} c_{NOx}(k) + \\ & \theta_{19} c_{NOx}(k-1)\end{aligned} \quad (13)$$

Finally this error estimation is calibrated on a dynamical test cycle and validated on a different cycle as shown in Fig. (5). For this validation already a simple NH_3 dosing control based on the assumption that the NO_x emissions

are consisting of 50% NO_2 and 50% NO is applied. Hence, the necessary NH_3 amount can be calculated easily with the information of (3) in which it is stated that two mol of NH_3 are necessary to reduce one mol of NO and NO_2. Although the slip is too high this control structure is suitable for the validation of the proposed model and the maximum NO_x reduction rate achievable with this SCR. In order to define a criterion for the estimation quality of the model FIT, VAF and the integral error (see Ljung [1999] and Stadlbauer et al. [2014]) are selected.

Table 1. FIT and VAF values for model validation

	FIT [%]	VAF[%]	e_{int}[%]
VAL(NO_x)	78	95	3.8
VAL(NH_3)	69	85	3.5

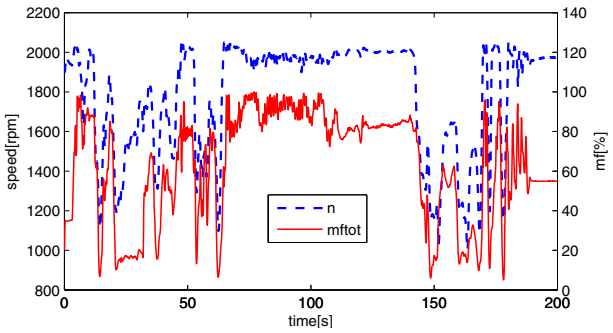

Fig. 5. Test cycle for validation and NMPC control

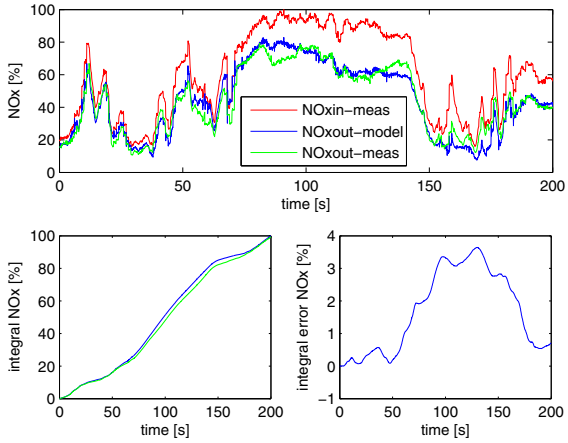

Fig. 6. Validation of the NO_x emissions of the SCR model

As it is indicated in Tab. (1), Fig. (6) and Fig. (7) in general a satisfying model for the NH_3 and the NO_x concentrations after the SCR, applicable for both SCR control and as simulation tool for NH_3 slip and reduction rate prediction, is achieved. Nevertheless as shown in Fig. (7) not all phenomenas (e.g. around 100s) can be covered perfectly by the proposed model.

3. NONLINEAR MODEL PREDICTIVE CONTROL

After the determination of the nonlinear SCR model a nonlinear NH_3 dosing amount control is proposed. The general targets of this NMPC control applied to the SCR

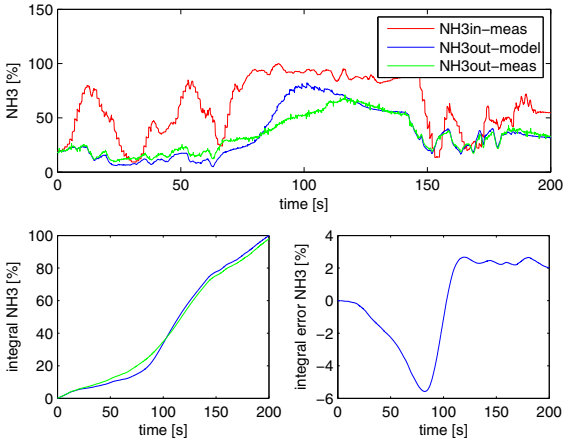

Fig. 7. Validation of the NH_3 emissions of the SCR model

are on one hand the reduction of up to 90% of the NO_x emissions (see Johnson [2013]) and on the other hand ammonia slip above 10ppm has to be avoided under any circumstance. Additionally the control scheme should work with the same performance under stationary as well as dynamically conditions such as during demanding transient cycles.

In order to implement the nonlinear model predictive control for the NH_3 dosing application, first a suitable reference has to be evaluated. Due to the fact that the NH_3 injection should be appropriate for the NO_x emissions, under the assumption that only NO/NO_2 with equal ratios can be reduced by the fast reaction, in principle the NO_x value may be a suitable option which can be found in literature as one of the most common approaches. Nevertheless not only the NO_x but also the ratio between NO and NO_2 has to be measured which makes it necessary to include an additional sensor or a virtual sensor concept (Stadlbauer et al. [2014]). In the case of the NO_x based ammonia injection always the optimal NH_3 amount based on the actual emissions is injected. It has to be considered that also the injected NH_3 needs a certain time to adsorb in the SCR to be available for the NO_x reduction. So during a dynamical test cycle it may happen that even if the dosing is accurate for actual emissions the adsorption is too slow and the possible reduction rate is not achievable due to an insufficient amount of adsorbed ammonia.

Therefore an interesting alternative to the NO_x reference approach is the control of the NH_3 storage, which assumes that always a filling level of 50% of adsorbed ammonia is stored in the SCR. This amount of adsorbed ammonia would be directly available during dynamical load changes and the SCR would be able to reduce the NO_x emissions still in an efficient way. However, also with this approach the tracking performance has to be defined appropriate to avoid slip and guarantee high NO_x reduction rates.

3.1 General NMPC problem formulation

The class of systems considered in this work is based on a nonlinear differential equation formulation with measured disturbances and restrictions on the inputs. For the design of the NMPC only the nominal model is considered and combined with an objective function penalizing the

tracking error and the control effort. As known, the determination of the control action in MPC and NMPC is formulated as optimization problem, where the values of u_k during the control horizon n_{CH} have to be determined and the objective function is calculated over the prediction horizon n_{PH}. This optimization problem can be stated as

$$\begin{aligned}
&\min_{u_k} \frac{1}{2} \sum_{k=0}^{n_{PH}} (y_k - y_{ref,k})^T Q (y_k - y_{ref,k}) + \Delta u_k^T R \Delta u_k \\
&s.t.\ u_k = u_{k-1} + \Delta u_k \\
&\quad x_{k+1} = f(x_k, u_k) \\
&\quad y_k = C_p x_k \\
&\quad \underline{u} \le u_k \le \overline{u} \qquad k = 0 \dots n_{CH} - 1 \\
&\quad \Delta \underline{u} \le \Delta u_k \le \Delta \overline{u} \quad k = 0 \dots n_{CH} - 1 \\
&\quad \Delta u_k = 0 \qquad k = n_{CH} \dots n_{PH}
\end{aligned} \tag{14}$$

where the tracking error is weighted by Q and the actuator advance is penalized by R.

3.2 Application to the SCR control

As next step the selected control structure (see Fig. 8) is applied to the 3 cell SCR model. As model states θ_1, θ_2, θ_3, e_{NOx} and e_{NH3} are implemented and as outputs, which are optimized (y_k), only the filling levels of the SCR are chosen. Moreover also the additional outputs of the model the NH_3 slip and the NO_x level at the outlet of the SCR are accessible and utilized for the evaluation of the method.

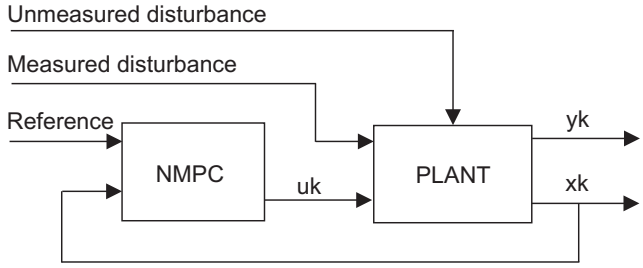

Fig. 8. Control structure of the NMPC

As measured disturbances the additional inputs which cannot be accessed by the control scheme are considered, which are in this case the NO_x emissions at the SCR inlet, the temperature of the SCR and the exhaust mass flow. These inputs were measured previously on the test bench of the institute to provide test data which is as close as possible to the real application. Due to the fact that there is already a model plant mismatch, in this simulation study no additional unmeasured disturbance is added and as control input directly the NH_3 injection is used.
The input constraints for the NH_3 (uk) dosing are set to 0 respectively 300mg/s, which is the maximum dosing amount of NH_3 at the test bench. Because the NH_3 dosing is done in a liquid form with Adblue a map calibrated by Adblue vaporization tests is necessary to calculate the gaseous available NH_3 in mg/s. Apart from that the sampling time Ts of the discrete NMPC formulation is fixed to 0.1s and the prediction horizon was set to $n_{PH} = 20$. Typically for MPC implementations, only the first of the 20 optimized control outputs is applied to the plant and in the next sampling time instant the optimal control problem is solved.
After these general definitions also the reference of the filling level and the tracking performance stated by the matrices Q and R has to be considered. Since for this control the most critical issue is to avoid NH_3 slip but also achieve high NO_x conversion rates it seems intuitive that during dynamical test cycles the filling of the first cell should never reach a filling level above 50%. The idea is, to still have remaining storage capacities left in the same instant also the second cell should be always filled with 50% to have enough adsorbed ammonia accessible if high emission peaks are occurring. Additional, as shown in Fig. 3, the filling levels of the three cells are not completely independent from each other which is a consequence from the assumed structure. Motivated by these considerations the reference of cell one and two are set to 50% and for cell three to 0%.

$$y_{ref,k} = [0.5\ 0.5\ 0] \tag{15}$$

Due to this dependency also the weighing factors of Q and R listed in (16),

$$Q = 10^{-6} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad R = 10^{-7}\,[5] \tag{16}$$

are chosen accordingly to avoid ammonia slip at the outlet of the SCR.

4. RESULTS

The SCR NMPC control scheme is finally applied to the same dynamical test procedure as illustrated in Fig. (5). Instead of the NH_3 dosing strategy based on the NO_x values, as described in chapter (2.3), the NMPC is based on the filling level of the SCR.

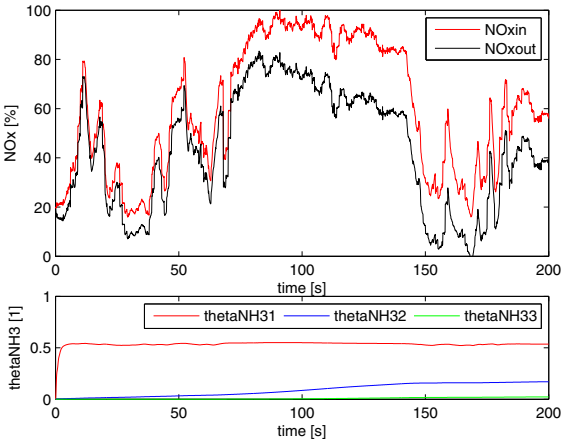

Fig. 9. NMPC SCR-control NO_x emissions and filling level

If a comparison between the results of the NO_x based SCR control shown in Fig. (7) and the results of the NMPC control (see Fig. (10)) is made, it is obvious that the NH_3 slip can be reduced drastically while the reduction rates achievable for the NO_x (depicted in Fig. (6) respectively Fig. (10)) remain on a similar level. Although the NH_3 dosing used during model estimation and NMPC

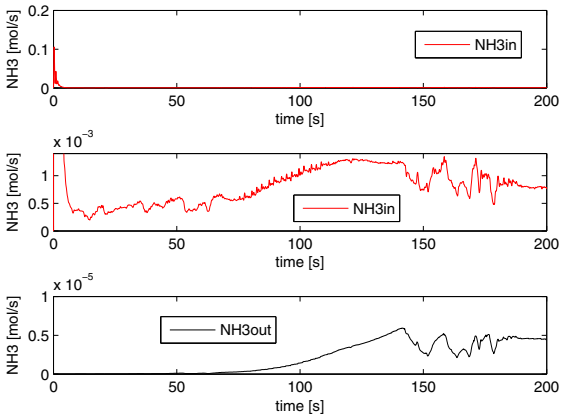

Fig. 10. NMPC SCR-control NH_3 input and NH_3 slip (subfigure 2: zoomed NH_3 injection)

cannot be compared directly, because the purpose of both approaches is too different, still the desired main goal to reduce the NO_x emissions as much as possible under the restriction that no NH_3 slip occurs is achieved. This is an important observation because although no slip and an overall reduction of 30% is achievable it is not the result what would be expected with a NO_x reduction of at least 80% in the ideal case (see Johnson [2013]). But in this case the reduction rate is limited by the choice of the SCR (length and volume) and fact that only NO and NO_2 with the same ratio can be reduced sufficiently fast. Moreover the desired dosing levels cannot be achieved which can be explained by two reasons. On one hand first all of the injected NH_3 is consumed by the first cell to reach the desired filling level of 50% and so there is a physical limitation for the second and third cell at the beginning. On the other hand it is limited by the conservatively chosen weighing factors to make sure that slip is avoided under any circumstance.

5. CONCLUSION

Within this work a nonlinear predictive control is developed to address the reduction of the ammonia slip under dynamic driving conditions in a DOC-DPF-SCR after treatment system. This is achieved by a converse approach to the common NO_x based strategies, namely a filling control based on a nonlinear SCR model. Due to the fact that the ACADO toolkit was used for this control no restrictions concerning the real time application on a test bench are uprising, as this toolkit provides a generator for c-code which can be implemented directly on a real time system. Although the results of this NH_3 control strategy are currently only available in simulation the promising results and the fact that the SCR model captures the real SCR behavior well, also for the test bench application a similar result is expected. Nevertheless the plant model mismatch has to be considered in real time simulation and evaluated in detail.

ACKNOWLEDGEMENTS

This work has been carried out at LCM GmbH and the JKU Hoerbiger Research Institute for Smart Actuators (JHI) as part of a K2 project. K2 projects are financed using funding from the Austrian COMET-K2 program. The COMET K2 projects at LCM and JHI are supported by the Austrian federal government, the federal state of Upper Austria, the Johannes Kepler University and all of the scientific partners which form part of the K2-COMET Consortium.

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