Master Thesis

Modelling of a Selective Catalytic Reduction (SCR) System for a Heavy-Duty Diesel Engine and Development of an Optimal Dosing Policy

Author: Uwe Schimatzek
Supervisor: Univ.-Prof. DI Dr. Luigi del Re
Dipl.-Ing. Patrick Schrangl
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Abstract

Increasing traffic density, especially in urban areas, and the associated stricter exhaust gas standards are important reasons for car manufacturers to put more effort in the development of exhaust gas aftertreatment systems. However, quantities such as engine power or fuel consumption must not be affected.
Nitrogen oxide emissions represent an essential component of the harmful exhaust products of internal combustion engines. These lead on the one hand to negative effects in the human respiratory system and contribute on the other hand significantly to the depletion of ozone. For this reason, so-called SCR (Selective Catalytic Reduction) systems have been developed, which aim at minimizing these emissions.
The aim of the present work is to determine and evaluate the optimization potential of nitrogen oxide emissions for the fulfilment of current and future emission standards. For this purpose, a model is first developed which simulates the real behaviour of the SCR system as accurately as possible, on the condition that the model is not too complex in order to keep the computational effort for simulation and control design low. This model is subsequently identified and validated with the aid of measurement data acquired on the real system.
Based on this model, an optimal urea solution dosing strategy is then calculated, which leads to reduced nitrogen oxide emissions compared to the ECU (engine control unit) strategy. This optimal policy is calculated for the test cycle of the Euro VI standard, the World Harmonized Transient Cycle (WHTC), using dynamic programming.

SCR Model

The idea behind this model approach is to interpret the SCR catalyst as an NH_3 storage device which has to be filled up to a certain level so it can convert the NO_x to non harmful water and nitrogen using the stored NH_3, based on the basic SCR reactions:

$$4NH_3 + 4NO + O_2 \rightarrow 4N_2 + 6H_2O \tag{1}$$

$$2NH_3 + NO + NO_2 \rightarrow 2N_2 + 3H_2O \tag{2}$$

$$8NH_3 + 6NO_2 \rightarrow 7N_2 + 12H_2O \tag{3}$$

and the oxidation of NO to NO_2:

$$2NO + O_2 \rightarrow 2NO_2 \tag{4}$$

The reaction rates of the stated processes are given by the following equations:

$$R_{st} = K_{st} \cdot e^{-\frac{E_{st}}{R \cdot T}} \cdot \frac{1}{V^2} \cdot n_{NH_3,free} \cdot n_{NO} \cdot n_{O_2} \tag{5}$$

$$R_{fast} = K_{fast} \cdot e^{-\frac{E_{fast}}{R \cdot T}} \cdot \frac{1}{V^2} \cdot n_{NH_3,free} \cdot n_{NO} \cdot n_{NO_2} \tag{6}$$

$$R_{NO_2} = K_{NO_2} \cdot e^{-\frac{E_{NO_2}}{R \cdot T}} \cdot \frac{1}{V} \cdot n_{NH_3,free} \cdot n_{NO_2} \tag{7}$$

$$R_{ox} = K_{ox} \cdot e^{-\frac{E_{ox}}{R \cdot T}} \cdot \frac{1}{V} \cdot n_{NO} \cdot n_{O_2} \tag{8}$$

which lead to the following dynamic equations of the model:

$$\dot{n}_{NH_3,free} = n^{\star}_{NH_3,free} - 4 \cdot R_{st} - 2 \cdot R_{fast} - 4 \cdot R_{NO_2} - n^{\star}_{NH_3,out} \tag{9}$$

$$\dot{n}_{NO} = n^{\star}_{NO,in} - 4 \cdot R_{st} - R_{fast} - 2 \cdot R_{ox} - n^{\star}_{NO,out} \tag{10}$$

$$\dot{n}_{NO_2} = n^{\star}_{NO_2,in} - R_{fast} - 3 \cdot R_{NO_2} + R_{ox} - n^{\star}_{NO_2,out} \tag{11}$$

$$\dot{n}_{O_2} = n^{\star}_{O_2,in} - R_{st} - R_{ox} - n^{\star}_{O_2,out} \tag{12}$$

The unknown parameters $(K_{st}, K_{fast}, K_{NO_2}, K_{ox}, E_{st}, E_{fast}, E_{NO_2}, E_{ox})$ were identified by iteratively solving the optimization problem:

$$\hat{\phi} = \underset{\phi}{\operatorname{argmin}} \sum_{k=1}^{N} (c_{NO_x,out,meas}(k) - c_{NO_x,out}(k))^2 \tag{13}$$

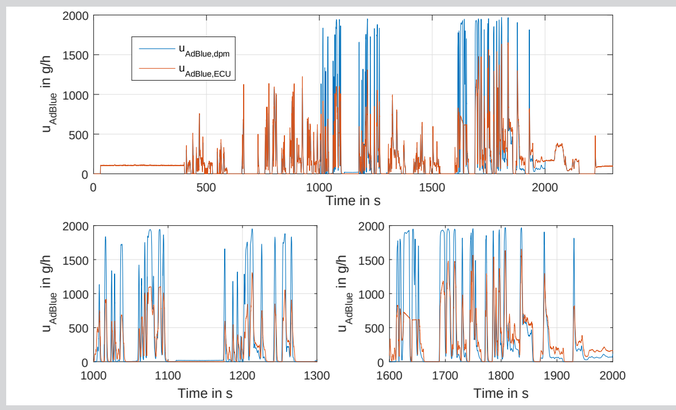
For the validation process, not only an experiment consisting of steady state operations of the engine was used, but also the WHTC to validate the model behaviour during transient processes.

Optimal Dosing Policy

Based on the developed model an optimal dosing policy was calculated for two segments of the WHTC using the method of dynamic programming (DP).
The DP algorithm evaluates the cost-to-go function $J_k(x^i)$ at every node in the disretized space by proceeding backward in time. The optimal control is determined by solving the optimization problem stated in equation 14 for each x^i at time index k.

$$J_k(x^i) = \min_{u_k} \left\{ h_k(x^i, u_k, w_k) + \Phi_k(x^i) + J_{k+1}(F_k(x^i, u_k, w_k)) \right\} \tag{14}$$

At each step of the optimization the function $J_k(x^i)$ is evaluated on grid points of the state variables, therefore, if the next state does not fall directly on a grid point, the value of $J_{k+1}(F_k(x^i, u_k, w_k))$ has to be evaluated approximately. There are several methods for this evaluation such as linear interpolation or using a nearest neighbour approximation. In the algorithm used, linear interpolation of the cost-to-go function is implemented. Once the backward calculation, with an optimal control signal map as its output, is done, this map is used to calculate the optimal control during a forward simulation starting at a given initial state x_0.

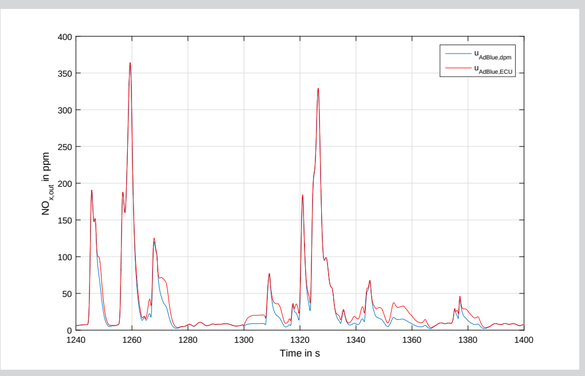


In general, the complexity of the DP algorithm is exponential in the number of state and input variables. Due to this fact, the computational effort of the *dpm* function was too large to calculate the optimal dosing policy for the whole 1800 seconds long WHTC. Hence, the optimal control law was determined for just two segments of the driving cycle.

Results

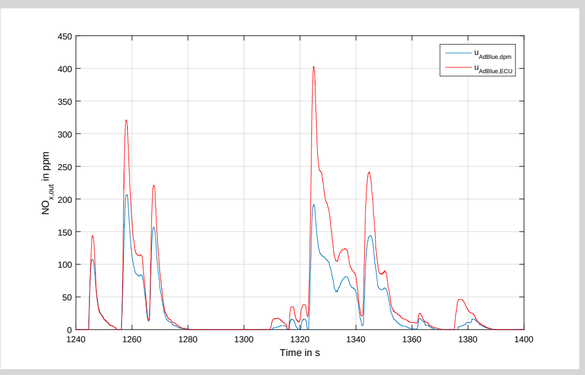
Simulation

In order to determine the effect of the optimal dosing policy on the nitrogen oxide emissions in simulation, this strategy was used as input for the model during the WHTC. This leads to the NO_x concentration at the outlet of the catalyst shown at the right which also illustrates the nitrogen oxide emission with the ECU dosing strategy as input for comparison. In order to generate a satisfying overview this figure shows just a segment of the experiment. This results in an improvement of 17.31% in the nitrogen oxide emission during the whole driving cycle which has a length of 2300 seconds.



Measurements

To receive the effect of the optimal dosing policy on the real system, this strategy was applied on the test bench to confirm the achieved improvement of the simulation. For this purpose, the WHTC was again executed on the test bench under the usage of the determined optimal AdBlue injection strategy. A comparison between the measurements (one with the ECU dosing and the second with the optimal dosing strategy) during a segment of the experiment is shown in the figure to the right. This leads to an overall amelioration of 20.96% during the whole driving cycle.



Conclusion and Outlook

Although the optimal dosing policy was calculated for just about 40% of the total time of the experiment an overall improvement over the ECU dosing strategy of 17.31% could be achieved in simulation. To confirm this improvement on the real system, the optimal dosing policy was implemented on the test bench and the experiment was executed again. This led to an amelioration of 20.96%.
The resulting nitrogen oxide emission by using the determined optimal dosing policy calculated with the DP algorithm can be used for example as a benchmark for future works on this topic. Thus, a developed controller can be evaluated on the basis of this benchmark to check if there is still potential in the control design. Another investigation based on this work could be the calculation of an optimal dosing policy for the whole test cycle for an even better benchmark. This task, however, would demand a very high computational effort which requires appropriate hardware with high computational power.