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Åberg, Andreas; Widd, Anders; Abildskov, Jens; Huusom, Jakob Kjøbsted

Published in:
IFAC-PapersOnLine

Link to article, DOI:
10.1016/j.ifacol.2017.08.1435

Publication date:
2017

Document Version
Publisher's PDF, also known as Version of record

Link back to DTU Orbit

Citation (APA):
Åberg, A., Widd, A., Abildskov, J., & Huusom, J. K. (2017). Methodology for Analysing the NOx-NH3 Trade-off for the Heavy-duty Automotive SCR Catalyst. IFAC-PapersOnLine, 50(1), 5998-6003. https://doi.org/10.1016/j.ifacol.2017.08.1435

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Methodology for Analysing the NOx-NH$_3$ Trade-off for the Heavy-duty Automotive SCR Catalyst

Andreas Åberg*, Anders Widd**, Jens Abildskov*, Jakob K. Huusom*

* CAPEC-PROCESS Research Centre, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Søltofts Plads, Building 229, DK-2800 Kgs. Lyngby, Denmark
** Haldor Topsoe A/S, Haldor Topsoes Allé 1, DK-2800 Kgs. Lyngby, Denmark

Abstract: This paper presents a methodology where pareto fronts were used to analyse how changes in the control structure for the urea dosing to the automotive SCR catalyst can improve the trade-off between NOx slip and NH$_3$ slip. A previously developed simulation model was used to simulate the European Transient Cycle (ETC) with P, PI, PD, and PID controllers, combined with Ammonia-NOx-Ratio (ANR) based feedforward to control the urea dosing. Results showed that PI with feedforward performed best. It was also shown that combining feedback with feedforward performed better than only using feedback or feedforward.

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Keywords: Automotive control, Automotive emissions, SCR, PID control, Feedback control, Feedforward control, Pareto front.

1. INTRODUCTION

1.1 Background

Diesel engine exhaust gases contains several harmful substances. The main pollutants are carbon monoxide (CO), hydrocarbons (HC), particulate matter (PM), and nitrous gases such as nitrogen oxide (NO) and nitrogen dioxide (NO$_2$) (together NO$_x$). Reducing the emission of these pollutants is of great importance due to their effect on urban air quality, and because of new legislations (Fritz and Pitchon, 1997; R.M. Heck and R.J. Farrauto, 2001). In a modern EU VI exhaust gas treatment system for heavy duty applications, the exhaust gases are typically treated with four different catalysts: a Diesel Oxidation Catalyst (DOC) which oxidises HC and CO to H$_2$O and CO$_2$, and NO to NO$_2$, a Diesel Particulate Filter (DPF) which filters PM, a Selective Catalytic Reduction (SCR) catalyst which removes NO and NO$_2$, and an Ammonia Slip Catalyst (ASC) which removes excess ammonia (NH$_3$) before the gases are released to the atmosphere. A representation of the system and the effect each catalyst has on the composition can be seen in Figure 1. A promising and widely used technology for removing NOx is based on SCR, with NH$_3$ in the form of hydrolyzed urea as a reducing agent (P. Gabrielson, 2004). Challenges with this technology include dosing the appropriate amount of urea to reach sufficient NO$_x$ conversion, while at the same time keeping NH$_3$-slip from the exhaust system below the legislation. This requires efficient control. Closed loop control of the SCR catalyst has been studied extensively in literature (C. Schär et al., 2004; J. Hu et al, 2011; D. Y. Wang et al, 2008), and feedforward based controllers (J. Patchett et al., 2003; D. Seher et al., 2003). Problems with feedback control are for example cross-sensitivity of NH$_3$ in NOx-sensors, dynamics with greatly varying time constants in combination with a transient system, and time delay in the urea dosing system (F. Willems et al., 2007). The exhaust systems rarely has NH$_3$ sensors, making it difficult to use NH$_3$ based control.

The performance measure of a controller is its ability to meet the legislation. However if a controller meets legislation, it is difficult to compare controllers against each other. Due to the nature of the SCR catalyst, the evaluation is a trade-off between NOx slip and NH$_3$ slip. Contributions in literature often focus on optimising a single control structure for a given system, rather than a full analysis of how different control structures can improve the performance of the SCR catalyst. Using pareto fronts to graphically analyse the best possible trade-off between NOx slip and NH$_3$ slip for a given control structure, and how the trade-off can be improved by changing the control structure, can to the author’s knowledge not be found in literature.

1.2 Contribution

This paper presents a methodology to graphically analyse the trade-off between NOx slip and NH$_3$ slip for the automotive SCR catalyst. The methodology can be used to investigate how changes in the urea dosing control structure improves the trade-off performance. Pareto fronts are generated for P, PI, PD, and PID controllers, both with and without ANR based feedforward, by simulating the European Transient Cycle (ETC) with the model by Åberg et al (A. Åberg et al., 2016b). The performance gain or loss for different control structures is analysed graphically.
inputs were generated experimentally by running the ETC on a 11 L diesel engine.

2.2 Controllers

P, PI, PD, and PID controllers have been tested both with and without feedforward action. The feedforward action throughout this article is referring to NOx inlet measurement based feedforward, as in (6),

\[ u^{FF} = ANR \cdot \text{NOx}_{in} \]  

where \( u^{FF} \) is the calculated feedforward dosing, ANR is the predetermined Ammonia-NOx-Ratio, and \( \text{NOx}_{in} \) is the inlet NOx concentration. The controllers that have been tested can be formulated as

\[ u(t_k) = K_c \left( e(t_k) + \frac{T_i}{T_d} \sum_{i=1}^{T} e(t_k) + D(t_k) \right) + u^{FF}(t_k) \]  

where \( u(t_k) \) is the dosing of \( \text{NH}_3 \) in mol/m³ at time \( t_k \), \( K_c \) is the gain, \( T_i \) is the integral time, \( T_d \) is the time the cycle has been running, subscript \( k \) indicates the time, \( T_s \) is the sampling time, \( e(t_k) \) is

\[ e(t_k) = r - \text{NOx}_{conversion}(t_k), \]  

where \( r \) is the set point in NOx conversion, and \( D(t_k) \) is the derivative action given by (K. J. Äström and M. Murray, 2008)

\[ D(t_k) = \frac{T_d}{T_d + NT_s} D(t_k-1) - \frac{T_dN}{T_d + NT_s} (e(t_k) - e(t_{k-1})) \]  

where \( T_d \) is the derivative time, and \( N \) is the filtering factor. The expression in (7) represents all controllers that have been tested in this work. A P controller represents the scenario where \( T_i \rightarrow \infty \), \( T_d = 0 \), and \( ANR = 0 \). A PI controller is the case where \( T_d = 0 \), and \( ANR = 0 \). A PD controller is when \( T_i \rightarrow \infty \) and \( ANR = 0 \). A controller coupled with feedforward is the case where \( ANR > 0 \), and the same parameters as previously. The sampling time \( T_s \) was 1s. The set point \( r \) was set to 100 % conversion in all simulations.
The control problem in SCR monoliths is of a multi-objective nature due to the legislation which places limits on NOx slip, average NH\textsubscript{3} slip, and maximum NH\textsubscript{3} slip. The set of solutions to a multi-objective optimisation problem can be represented as a pareto front, which is the curve representing the solutions that are pareto efficient. Here, pareto fronts were used to present the trade-off between NOx slip and NH\textsubscript{3} slip for different controllers.

The process of producing the pareto fronts is shown in Figure 2. A controller is selected for testing, for example a P controller. The ETC is simulated using the controller with a certain $K_c$ parameter. The cycle performance is evaluated, and the results are saved. This represents one data point on the pareto front. The process is repeated with new $K_c$ parameter, until a pareto front is complete. For controllers that have several parameters, such as a PI controller, the pareto fronts were generated using the same procedure, but for a certain $T_i$. A range of $T_i$ values were tested and pareto fronts for each $T_i$ were produced by simulating the cycle for a range of $K_c$ values, and the influence of $T_i$ was therefore evaluated. The parameter values for $K_c$, $T_i$, and $T_d$ that has been used are based on values that gave reasonable performance. The performance was evaluated using the NOx slip in g/kWh for the entire cycle, and the average NH\textsubscript{3} slip in vol-ppm. The NOx mass was calculated by assuming that all NOx is NO\textsubscript{2}. The average NH\textsubscript{3} slip was calculated by taking the mean of all NH\textsubscript{3} outlet concentration measurements. After the pareto fronts are generated a visual representation of the tested configurations of a control structure is achieved. This can be used to see which controller satisfies the legislations. It also enables comparisons between controllers, as it becomes clear if a control structure outperforms another structure. The benefit of the analysis is that the conclusions on control structure should be independent of the size or activity of the monolith. The qualitative results should also be independent on parameters such as engine size, and ambient conditions. The pareto fronts are in most cases cropped, to present relevant results. The pareto fronts presented here have a higher NH\textsubscript{3} slip and lower NOx slip than is typical for a monolith of this size. This is done because the differences between the controllers is more clear at lower NOx slip, and the qualitative results remain the same.

The commercial software Matlab was used for simulation. The simulated monolith was a full body vanadium based catalyst with 270 CPSi on a corrugated substrate, 12.7 inches long and 9 inches diameter. The engine was a 10 liter engine without EGR, following the ETC. For each pareto front 40 simulations were performed, where each took approximately 500 s. The initial conditions for each simulation was the end result of the previous simulation. For the first simulation in a series, the simulation was performed twice to achieve realistic initial conditions.

3. RESULTS AND DISCUSSION

This section will present the pareto fronts for P, PI, PD, and PID controllers, both with and without feedforward.

3.1 P-control

The P controller has one free parameter, the gain $K_c$. Figure 3 shows the pareto fronts for P controllers with varying degrees of feedforward, ranging from ANF = 0 to ANF = 1.5. It can be seen that the controller with ANR = 0 starts to increase in average NH\textsubscript{3} slip rapidly after the NOx slip goes below 3 g/kWh. The EURO IV emission limited the NOx slip to 3.5 g/kWh, and it appears that a P controller was enough to meet the previous emission limits, at least with the assumptions included in this work. As the feedforward is increased it can be seen that the pareto front is shifted inwards, giving a better trade-off between NOx and NH\textsubscript{3}. When ANR > 1, meaning that more NH\textsubscript{3} than NOx is dosed, the pareto fronts are shifted upwards, and the feedforward that should be used depends on the required NOx slip.

3.2 PI-control

The PI controller has two free parameters, the gain $K_c$ and the integral time $T_i$. Figure 4 shows the influence of the integral time for a PI controller without any feedforward. As seen, the difference in the cycle based performance for different $T_i$ is small. The transient ETC ensures that the process is never in steady state, and it makes little difference if the integral action is acting towards a hypothetical steady state in 60s or 70s. Figure 5 shows the pareto fronts for a PI controller with ANR = 0, and ANR = 0.9-1.2. It can be seen that as with the P controller, introducing feedforward improves performance. The overlap between controllers when the feedforward is increased...
Toulouse, France, July 9-14, 2017
Proceedings of the 20th IFAC World Congress

K evaluated, and the results are saved. This represents one cycle, and the average NH$_2$.

Pareto Fronts
general trends of the pareto fronts will be the same.

mass was calculated by assuming that all NOx is NO.

PI controller, the pareto fronts were generated using the

Figure 2. A controller is selected for testing, for example

The process of producing the pareto fronts is shown in

T, and c that has been used are based on

formly distributed to the catalyst. It was also assumed

that the urea was decomposed instantly to NH$_3$.

slip in vol-ppm. The NOx

an engine.

conclusions on control structure should be independent of

another structure. The benefit of the analysis is that the

tested configurations of a control structure is achieved.

T, and c

d

that should also be independent on parameters such as engine

size, and ambient conditions. The pareto fronts are in

shoulder between NOx and NH$_3$.

slip, and maximum NH$_3$.

between NOx slip and NH$_3$.

slip. The set of solutions to a multi-objective optimisation

mass will be saved and in the next step evaluated for

slip, and NOx and NH$_3$.

slip goes below 3 g/kWh. The EURO IV emission

simulation was the end result of the previous simulation.

took approximately 500 s. The initial conditions for each

was introduced to the ETC. The initial conditions included

the ETC, with different levels of ANR feed forward. Legend:

ANR = 0 ( ), ANR = 0.2 ( ), ANR = 0.5 ( ), ANR = 0.8 ( ), ANR = 0.9 ( ), ANR = 1.0 ( ), ANR = 1.1 ( ), ANR = 1.2 ( ), ANR = 1.4 ( ), ANR = 1.5 ( )

is more prominent with the PI controller than with the P

controller. Generally it seems better to increase the Kc parameter up to a certain level, instead of increasing the feedforward. When the feedback becomes too strong, increasing the feedforward is better for the NOx-NH$_3$

trade-off. The trade-off curves become increasingly steep as feedforward is increased, which is also seen with the P

controller. This is likely because of fundamental limits of the control structure, and the NOx slip can not become smaller than a certain limit. At ANR = 1.2 and beyond, increasing the feedback only gives an increase in NH$_3$ slip, while not reducing the NOx slip.

3.3 PD-control

The PD controller has three free parameters, the gain

Kc, the derivative time $T_d$, and the filtering factor $N$. Figure 6 shows several pareto fronts with different $T_d$

and N parameters. As can be seen the curves have an erratic shape and for a given $T_d$ and $N$, two different

Kc can give the same NH$_3$ slip and different NOx slip. (K. J. Åström and M. Murray, 2008) state that the $N$

parameter normally takes values between 8 and 20, which has been adopted here. The derivative time has also been tested in a broad range, with limited success. The PD controller performs worse than P controllers that were shown in Figure 3. To investigate if the reason for the erratic shape was a too strong derivative action, the gain

was held constant while increasing the derivative time, in Figure 7.

It can be seen that even for low derivative times, the trade-off curve became irregular and no smooth shape.
was obtained. The reasons for this behaviour is unknown, however we suspect that even though the signal was considered noise free, the transient input resulted in a rapidly changing error, that the derivative action was sensitive to. The fact that the results showed cases where the controller gave the same NH3 slip for different NOx-slip, suggests there are periods where one parameter set results in a large NH3 slip at a certain time, while the other parameter set does not. Because of these results and the fact that the PD controller performed worse than a P controller even for good parameters, it was decided not to look further into these problems, and abandon the PD controller from further consideration.

### 3.4 PID-control

The PID controller has four free parameters, the gain $K_c$, the integral time $T_i$, the derivative time $T_d$, and the filtering factor $N$. $T_i$ was chosen as the value that showed the best performance during PI analysis in section 3.2, and $T_d$ and $N$ were chosen based on performance in PD analysis in section 3.3. Figure 8 shows pareto fronts for PID controllers with ANR = 0, and ANR = 0.7-1.1. It can be seen that the negative effect of derivative action seems to have disappeared. If it is improving performance cannot be concluded until it is compared with the PI controller in section 3.5. The performance is, as with the P and PI controller, improved when feedforward is included. The overlap seen previously when feedforward is increased is also seen here.

#### 3.5 Comparison

Figure 9 compares some of the previous results. The best controller tested was the PI with feedforward ANR = 1.0. This controller outperformed the P controller with feedforward, meaning that the integral action increased performance when combined with feedforward as well. The difference between a P controller and a PI controller was however substantially bigger without feedforward. The reason integral action improves performance even though no steady state is reached it is because it ensures that there is continuous dosing, even during periods of low error. The effect of feedforward was dominating, and as can be seen, a P controller with feedforward outperformed a PI controller without feedforward. The difference between a PI controller and PID controller without feedforward is difficult to see in Figure 9. However if zoomed, it can be seen that the PI controller was slightly better than the PID controller. This confirms that the derivative action has little or no effect at the expense of added complexity, also combined with other parts. Figure 9 shows that controllers including both feedback and feedforward performed better than controllers with only feedforward. This shows that even though the feedforward was dominating, the feedback control action contributes to the cycle based performance.

### 4. DISCUSSION

The presented methodology provides a way to compare controllers graphically in their whole operational span. Although it has only been applied to P, PI, PD, and PID controllers with feedforward in this work, it can be applied to other controllers as well, for example model based controllers, controllers based on NH3, etc. For a controller that requires an optimisation problem to be solved, it is suitable if the user is uncertain about the weights that should be used in the objective function. If the objective function weights are changed and the controller is solved, it is suitable if the user is uncertain about the weights that should be used in the objective function. If the objective function weights are changed and the controller is solved, it is suitable if the user is uncertain about the weights that should be used in the objective function. If the objective function weights are changed and the controller is solved, it is suitable if the user is uncertain about the weights that should be used in the objective function.
represent the maximum peak slip, or expanded so that all three legislative limits are covered. NH₃ consumption can also be included as a criteria in the optimisation problem. Addition of sensor noise or cross sensitivity can also be added to the model, thereby giving a more realistic controller performance.

The results are general in the sense that changes in catalyst volume or other system parameters would change the quantitative results but not the qualitative. This has been confirmed in simulations not shown here, where the pareto fronts for the P and PI controllers were plotted for two different volumes. As expected, the larger volume improves the trade-off between NOx slip and NH₃ slip, since more catalyst is available for reaction.

The study shows that out of the tested control structures, the feedforward is important for the overall performance. Sensors before the SCR catalyst are therefore recommended. It is possible to use an engine-NOx map that provides information about the engine outlet NOx levels for different driving conditions. This however suffers from some problems, such as not taking ambient conditions into account.

5. CONCLUSIONS

This paper has presented a methodology to analyse the trade-off between NOx slip and NH₃ slip for the automotive SCR catalyst by using pareto fronts. The methodology was applied to P, PI, PD, and PID controllers both with and without ANR-based feedforward. It was shown that the PI controller with feedforward included gave the best trade-off. It was also shown that there is a performance increase in combining feedback with feedforward compared to using either one alone.

ACKNOWLEDGEMENTS

The financial support from Innovation Fund Denmark under grant number 103-2012-3 is gratefully acknowledged.

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