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Ammonia injection optimization for SCR aftertreatment systems

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Abstract

This work presents an optimized ammonia injection strategy for the Worldwide Harmonized Light Vehicles Test Cycle (WLTC) and its potential benefits in terms of NO_x emissions and ammonia consumption in the selective catalytic reduction (SCR). An optimization tool based on optimal control was used to improve the ammonia injection in the SCR with different NO_x emissions limits. This optimal control can be used in two ways: one to minimise NO_x emission and another to reduce the ammonia consumption in the SCR. The optimized strategy, as well as the standard ammonia injection strategy, were tested and compared on a fully instrumented engine test bench when applied in a WLTC cycle. The results showed a considerable improvement with the use of the optimization tool. When compared to the standard calibration, the new injection strategy for the same amount of ammonia injection reduced NO_x emissions by 13.7%, and for the same NO_x concentration emissions 33.5% of ammonia consumption was saved.

Keywords

Selective catalytic reduction, Engine aftertreatment, Vehicle emissions

Introduction

According to the latest report released by the International Energy Agency (IEA) in the World Energy Outlook 2018 (WEO), the power demand for transportation sector will grow 63% until 2040[1]. Since most of the powertrains are based to some extent (even in the case of Hybrid Electric Vehicles) in internal combustion engines (ICE), one may expect a substantial increase in fuel consumption and emissions during following decades. Modern Diesel engines with low specific fuel consumption and high-power output[2] are an attractive choice in the light duty, but specially in the medium to high duty vehicle markets to reduce fuel consumption and CO2 emissions. However, due to the nature of compression ignition combustion process, emissions and particularly NO_x emissions are an issue of Diesel engines. To cope with them, in the last years emission regulations have become more and more strict (even for the shipping field[3]). Emissions limits have been considerably reduced and the driving cycles to assess the vehicle emissions have become more aggressive (Worldwide Harmonized Light Vehicles Test Cycle - WLTC) and more general (Real Driving Emissions - RDE), covering a wider range of operating conditions. In addition, the use of On-Board Diagnostics (OBD) has been mandatory since 1996[4] and regulations require the monitoring of the aftertreatment system for malfunction[5] and performance degradation[6].

Amongst aftertreatment systems, the selective catalytic reduction (SCR) is currently one of the most widespread devices[7] since it is able to reduce the NO_x emissions up to 95%[8]. SCR aftertreatment is presented in the most diverse approaches to reduce NO_x emissions. Kojima *et al.*[9] presented the benefits of the SCR coated on diesel particulate filter (DPF) in terms of NO_x efficiency, soot performance and packaging. Saari *et al.*[10] evaluated the performance of SCR aftertreatment system for heavy duty truck operating in real-world conditions, finding the average NO_x emissions 0.05 g/kWh above the Euro IV emission limits in transient tests. Prikhodko *et al.*[11] evaluated the passive SCR concept for lean gasoline NO_x control, achieving a 10% benefit in fuel consumption optimizing the rich air-fuel equivalence rate and ignition time. And Liang *et al.*[12] used a 1D SCR model to conduct the compact structure design of the SCR system and the effect of structural parameters on SCR performance, as well as the optimization of these parameters, reducing the SCR volume by 23.82%, the pressure drops generated by SCR reactor by 10.38% and the conversion of NO_x by 0.51%. Lin *et al.*[13] developed an integrated SCR-AMOX control-oriented model to decouple the NO_x and ammonia (NH_3) concentrations from the NO_x sensor signal, achieving a 95% NO_x estimation error less than 28 ppm and 80% of the NH_3 error lower than 5 ppm.

Measures to improve the performance of SCR systems focus on:

- Improving design and integration: reducing their volume, providing packaging flexibility as well as closer placement of the SCR catalyst to the engine for faster light-off (i.e, temperature at which catalytic reactions are initiated)[14]. Increasing the injection pressure that affects the atomization process and produces smaller particles at higher speeds, promoting

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wider overall spray angles and that when combined with a high temperature mass flow can improve the evaporation and mixing process in the SCR system[15].

- Improving its control and diagnosis: SRC catalyst reduces the NO_x concentration in the presence of ammonia (NH_3) so an injection of such a substance is required. One of the characteristic issues of the SCR is its slow dynamics. In particular, it is not possible to reduce the NO_x concentration by injecting an equivalent amount of NH_3 at a given time, the characteristic times of adsorption, desorption and chemical reactions in the SCR require certain amount of NH_3 previously stored in the SCR to effectively reduce NO_x. Once NH_3 is adsorbed on the surface of the catalyst, it is ready to react with the NO_x present. Note that the catalyst has not capacity to retain NO_x, so that if there is not enough NH_3 storage, these NO_x will be released[16] as slip. On the contrary, if the amount of NH_3 stored in the SCR exceeds its maximum capability NH_3 will not be retained. NH_3 slip is the ammonia injected into the SCR but not consumed by the reduction reaction[17]. As the EURO VI for heavy duty limits NH_3 emissions by 10 ppm, ammonia injection must be accurately controlled: excess leads to NH_3 slip and little decreases the NO_x conversion efficiency[18]. In this sense, this situation is doubly undesirable since wasting NH_3 has an economic cost and its emission to the environment is harmful. Accordingly, a proper ammonia injection strategy translates into both cost and emissions. Due to previous reasons, SCR control is a challenging problem currently addressed by many authors and research groups, as Jiang *et al.*[19] which used a data driven modeling with a finite impulse response filter to replace the use of physical sensors in the SCR catalyst NO_x and NH_3 input measurements, Soleimani *et al.*[20] presents a review of the state-of-the-art and the reliability challenges of the aftertreatment system and Pezzini *et al.*[21] shows a diagnostic methodology for fault detection in different aftertreatment systems.

In this context, as the SCR is a complex dynamic system interacting with other systems and phenomena in the ICE[22], the performance of a given design is strongly affected by the control strategy used. Moreover, one may find that the control strategy or even calibration performing well for a given SCR may provide negative outcomes with a different design[23]. In this sense, it is useful to have a fair basis for comparison of the design and controls of the SCR. Advances in computation capabilities made Optimal Control (OC) theory attractive to optimize complex dynamic system[24,25]. The OC theory was introduced by Lev Pontryagin and Richard Bellman, and a more detailed explanation of the subject can be found in their work.[26,27]. OC theory is a model-based control approach where different mathematical methods are used to calculate the controls that must be applied to a system to minimise a predefined cost index[28]. In this sense, OC is a suitable tool to provide a fair basis for comparison since will lead to the best possible performance of any SCR assessed. Accordingly, the purpose of this paper is to obtain by means of OC the optimal trajectory in the ammonia injection that minimises its consumption provided a NO_x limit. The final objective of this optimization is providing a best case scenario for comparison with other SCR designs and provide basis for the SCR control strategy optimization. The application of OC is based on three main aspects:

- The problem description: In this case the WLTC has been considered as it is the actual type-approval test in the european light duty market, and the objective of the optimization has defined as minimising the ammonia injector subject to different NO_x restrictions.
- Modelling: To compute the optimal ammonia injection strategy, a model able to estimate the impact of control decissions in the performance of the SCR is needed[29]. The modelling process is a compromise between using as much mathematical complexity as necessary to describe correctly the phenomena while keeping the model as simple as possible. Regarding the aftertreatment modeling, three transport process are described in the catalyst surfaces: mass transfer, heat transfer and momentum transfer[30]. Mora *et al.*[31] In this study, a zero-dimensional (0D) control-oriented SCR chemical model is applied, which considers the NH_3 storage and NO_x main reaction. This model is based on the Continuously Stirred Tank Reactor (CSTR) approach (i.e, that is, the concentration of one gas species is homogeneous in all the directions[32]) in order to compute the NO, NO_2 and NH_3 balances.
- Optimization tool: Despite keeping simplicity, the model complexity needed to reproduce de behaviour of an SCR in a dynamic cycle like the WLTC leads to a number of states that make the computational cost of global optimization methods such as Dynamic Programming (DP) prohibitive. For this reason an implementation of a Direct Method (DM) has been preferred in this work. The DM is a family of OC methods based on transcribing the OC problem into a large but sparse non-linear programming (NLP) problem[25].

The paper is structured as follows: The facilities and experimental apparatus are presented in Section 'Experimental setup'. Then, the 0D model methodology and optimization approach are presented in Section 'Methodology', followed by Section 'Results and discussion'. Finally, 'Conclusion' can be found in the last Section.

Experimental setup

The engine used in this work was a Euro 6 four-cylinder light-duty engine with high pressure Exhaust Gas Recirculation (EGR), Variable Geometry Turbine (VGT) and common-rail fuel injection system. Complementary engine information is shown in Table 1.

Table 1. Engine parameters

Displaced volume	1499 cm^3
Bore x Stroke	75 x 84.8 mm
Compression ratio	16.4:1
Maximum torque	300 Nm @ 1750 rpm
Maximum power	96 kW @ 3750 rpm
Emissions standard	Euro 6

In the exhaust line was placed a selective catalytic reduction system filter (SCRF), Table 2 shows the catalyst parameters.

Table 2. SCRF catalyst parameters

Diameter x length	0.07 x 0.3 m
Cell density	600 cpsi
Wall thickness	0.8 mm
SCR Storage Capacity	80 mol/m^3
Surface coverage	0.037431 [-]
Critical surface coverage	0.1995 [-]

The engine was coupled to an Horiba DYNAS3 asynchronous dynamometer. The dynamometer is controlled by Horiba SPARC integrated with HORIBA Automation System STARS. Configuration, parameterization and monitoring of the controller algorithms have been accessed in the STARS user interface. The dynamometer can be used for engine steady-state and dynamic testing. In particular, it is able to emulate vehicle behaviour to carry out engine in the loop tests simulating driving conditions with a Road Load Simulation (RLS) module.

An open Electronic Control Unit (ECU) was used to modify the SCR control strategy. For some relevant signals, a rapid prototyping system is connected via ECU ETK port allowing to send and receive signals. This bypass configuration is created by INTERCRIO and compiled in the dSpace system. The hardware setup is mainly composed of dSpace Microautobox II, ETAS 910 and open ECU.

For exhaust measurements, thermocouples and NO_x sensors were used before and after SCR, as well as a NH_3 sensor after SCR. An Horiba FTIR MEXA-ONE-FT Motor Exhaust Gas Analyzer was placed after the SCR and used to compare with the sensor measurements. The test bench is also equipped with a Horiba FQ-2100DP Fuel Consumption Measurement System and others conventional sensors (boost pressure, mass air flow, etc.). Table 3 shows the specifications of the pollutant measurement equipment. The complete experimental setup is shown in Figure 1.

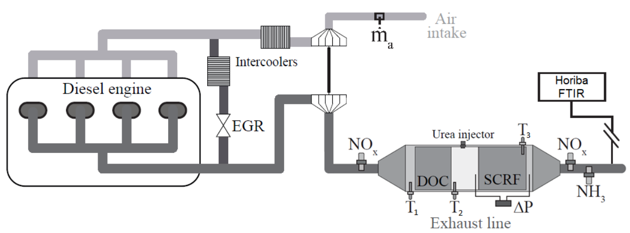

Figure 1. Experimental setup.

where m_a is the sensor that measures the air mass flow entering the engine, NO_x is the NO_x sensors, NH_3 is the ammonia sensor and T are the thermocouples.

Table 3. Equipment specifications

Equipment	Measurement
FTIR	NO_x 0-2000 ppm $\pm1.0\%$ of full scale NH_3 0-1100 ppm $\pm1.0\%$ of full scale
NO_xsensor	0-1860 ppm ±15 ppm @0-1000 ppm $\pm1.5\%$ @$\leq$1000 ppm
NH_3sensor	0-6550 ppm $\pm0.5\%$ of full scale

Regarding the test conditions, two sets of tests have been used in the present work. First a set of steady state tests covering the complete engine map have been tested with steps in the ammonia injection to identify the SCR model parameters. In a second step, a dynamic test, particularly the WLTC cycle has been tested to validate the model and assess the impact of different strategies on the NO_x emissions and ammonia consumption in conditions representative of actual driving.

Methodology

The aim of this work is applying OC techniques to find the SCR control strategy that minimises ammonia consumption with a specific limit for NO_x emissions. Despite the results obtained, OC cannot be applied for real time control since it assume perfect knowledge of the driving cycle, they can be used to evaluate the performance of a given SCR design or control strategy, and also to provide insight on the factors that an applicable control strategy should address. The first task to achieve the objectives is the development, identification and validation of the SCR model used to calculate the optimized ammonia injection. The second task is the implementation of the SCR model within an optimization tool that provides the optimal ammonia injection policy. The final task consists in applying the calculated SCR control policies to the actual engine in order to validate their performance. The previous tasks are presented in following subsections.

SCR model

The SCR model is based on the 0D model presented by Mora[33] and follows the standard control oriented modelling approach available in literature, where Shost *et al.*[34] presents an embedded control model of the SCR dosing system, Upadhyay and Nieuwstad[35] shows the modeling of a 0 dimensional SCR catalyst and Wu *et al.*[36] presents an ammonia injection control strategy under transient process. A general sketch of the model states, inputs and outputs is shown in Figure 2.

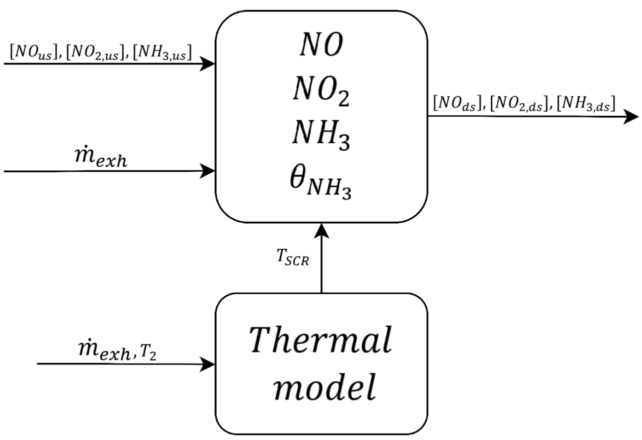

Figure 2. SCR 0D model scheme.

The model uses as input signals: nitrogen oxide (NO_{us}) and nitrogen dioxide ($NO_{2,us}$) from the engine exhaust gas, ammonia injected into the SCR catalyst ($NH_{3,us}$), exhaust mass flow ($\dot{m}_{exh}$) and temperature (T_{SCR}) of the model temperature, which in turn uses a filter on the temperature coming from the thermocouple placed in the middle (T_2) of the SCR catalyst. The model output signals are: nitrogen oxide (NO_{ds}), nitrogen diode ($NO_{2,ds}$) and ammonia slip ($NH_{3,ds}$), which in this case is the concentration of ammonia after reactions inside the SCR catalyst. Where the species concentration, temperature and exhaust mass flow are in mol/m^3, K and kg/s, respectively.

The reducing agent for NO_x reduction injected in the SCR catalyst is an aqueous urea solution (AdBlue) that is decomposed in NH_3. The used model does not include the urea decomposition and assumes that the available ammonia is a constant proportion of the urea injection (32.5%).

The model considers the main SCR reactions as well as the NH_3 adsorption, desorption and storage on the catalyst surface (θ_{NH_3}). The SCR reactions to compute the species balances of NO, NO_2 and NH_3 (i.e. standard, fast and slow reactions)[37], and NH_3 adsorption-desorption are calculated with the following Arrhenius equations, respectively.

The NH_3 reacts with NO, which accounts for most of the NO_x emissions in the raw exhaust of diesel engines. This reaction is referred to as the standard SCR reaction rate (r_{std})[38].

$$r_{std} = k_{std} e^{[\frac{-E_{std}}{R}(\frac{1}{T_{SCR}} - \frac{1}{T_{ref}})]}[NO]\theta^*_{NH_3}(1 - e^{(\frac{-\theta_{NH_3}}{\theta^*_{NH_3}})}) \quad (1)$$

where, k_{std} $[m^3/mol\ s]$ is the standard SCR frequency factor, E_{std} $[J/mol]$ standard SCR activation energy, R $[J/mol\ K]$ universal gas constant, T_{SCR} [K] SCR temperature, T_{ref} [K] reference temperature, NO $[mol/m^3]$ nitrogen oxide concentration and θ_{NH_3} $[-]$ surface covarage fraction. The parameter critical surface coverage ($\theta^*_{NH_3}$) $[-]$ has been included, since the standard reaction rate of SCR is essentially independent of ammonia surface coverage above a critical surface concentration of NH_3[39].

As diesel oxidation catalyst (DOC) or diesel particulate filter (DPF) systems, are installed prior to SCR, NO in the exhaust gas is oxidized to NO_2. With the production of NO_2, NH_3 reacts in the presence of NO and NO_2. This is called the SCR rapid reaction rate (r_{fst}) because it is the fastest of the major SCR reactions[40].

$$r_{fst} = k_{fst} e^{[\frac{-E_{fst}}{R}(\frac{1}{T_{SCR}} - \frac{1}{T_{ref}})]}[NO][NO_2]\theta_{NH_3} \quad (2)$$

where, k_{fst} $[m^6/mol^2\ s]$ is the fast SCR frequency factor, E_{fst} $[J/mol]$ fast SCR activation energy and NO_2 $[mol/m^3]$ nitrogen dioxide concentration.

Meanwhile, NH_3 may react with NO_2 alone. This is the slow reaction rate of SCR (r_{slw}) because the reaction occurs very slowly, slower than the major SCR reactions[41].

$$r_{slw} = k_{slw} e^{[\frac{-E_{slw}}{R}(\frac{1}{T_{SCR}} - \frac{1}{T_{ref}})]}[NO_2]\theta_{NH_3} \quad (3)$$

where, k_{slw} $[m^3/mol\ s]$ is the slow SCR frequency factor and E_{slw} $[J/mol]$ slow SCR activation energy.

The NH_3 adsorption (r_{ads}) and desorption (r_{des}) reaction rate equations are presented below.

$$r_{ads} = k_{ads} e^{[\frac{-E_{ads}}{R}(\frac{1}{T_{SCR}} - \frac{1}{T_{ref}})]}[NH_3](1 - \theta_{NH_3}) \quad (4)$$

$$r_{des} = k_{des} e^{[\frac{-E_{des}(1-\theta_{NH_3})}{R}(\frac{1}{T_{SCR}} - \frac{1}{T_{ref}})]}\theta_{NH_3} \quad (5)$$

where, k_{ads} $[m^3/mol\ s]$ is the adsorption frequency factor, E_{ads} $[J/mol]$ adsorption activation energy, k_{des} $[1/s]$ desorption frequency factor, E_{des} $[J/mol]$ desorption activation energy and NH_3 $[mol/m^3]$ ammonia concentration.

For the NH_3 storage, a standard mass balance is applied, so the accumulated NH_3 in a given instant depends on its previous state, adsoption, desorption and the consumption through different reactions with their corresponding stochiometry:

$$\frac{\partial \theta_{NH_3}}{\partial t} = r_{ads} - r_{des} - r_{std} - 2r_{fst} - 4/3 r_{slw} \quad (6)$$

In order to include the effect of spatial velocity (SV) of the exhaust gas flow (Eq. 7) of the NO, NO_2 and NH_3 and have the effect of the residence time of the species inside the catalyst the CSTR approach are used.

$$SV = \dot{m}_{exh}/\delta_{gas}/\zeta_{SCR}/V_{SCR} \quad (7)$$

where, $\dot{m}_{exh}$ [kg/s] is the exhaut mass flow, δ_{gas} $[kg/m^3]$ is the gas density, ζ_{SCR} $[-]$ is the factor that represents the open portion of the SCR volume, and V_{SCR} $[m^3]$ is the SCR volume. The species concentration states are presented in the following equations:

$$\frac{\partial NO}{\partial t} = -\Omega(r_{std} + r_{fst}) + SV([NO_{us}] - [NO]) \quad (8)$$

$$\frac{\partial NO_2}{\partial t} = -\Omega(r_{fst} + r_{slw}) + SV([NO_{2,us}] - [NO_2]) \quad (9)$$

$$\frac{\partial NH_3}{\partial t} = -\Omega(r_a - r_d) + SV([NH_{3,us}] - [NH_3]) \quad (10)$$

where, Ω $[mol/m^3]$ is the total ammonia storage capacity of the SCR catalyst.

To fully characterize the catalyst behaviour, it is necessary to estimate some parameters based on measured input-output data from an operational SCR catalyst[42]. If the temperature of the catalyst was too low or the initial value for the surface coverage was wrong, the estimated results may be affected. To minimise these errors and improve the 0D model a Design of Experiments (DoE) was used to identify the SCR model tunable parameters (i.e, for each parameter the maximum and minimum values were defined, after applying the DOE the combination of parameters that showed the smallest error between experimental and simulated were selected). Table 4 shows the estimated values for all parameters, including the

Table 4. SCR 0D model tunable parameters

Tunable Parameter	Symbol	Value
Adsorption frequency factor	k_{ads}	175 $[m^3/mol\ s]$
Desorption frequency factor	k_{des}	0.02 $[1/s]$
Fast SCR frequency factor	k_{fst}	3.39e4 $[m^6/mol^2\ s]$
Slow SCR frequency factor	k_{slw}	1.85 $[m^3/mol\ s]$
Standard SCR frequency factor	k_{std}	36 $[m^3/mol\ s]$
Adsorption activation energy	E_{ads}	11.47 $[J/mol]$
Desorption activation energy	E_{des}	1.11e5 $[J/mol]$
Fast SCR activation energy	E_{fst}	3.58e4 $[J/mol]$
Slow SCR activation energy	E_{slw}	4.75e4 $[J/mol]$
Standard SCR activation energy	E_{std}	3.14e4 $[J/mol]$

Parameter	Symbol	Value
Critical Surface Coverage	$\theta^*_{NH_3}$	0.1995 $[-]$
Gas Density	δ_{gas}	0.7327 $[kg/m3]$
Reference Temperature	T_{ref}	600 $[K]$
SCR Storage Capacity	Ω	80 $[mol/m^3]$
SCR Volume	V	0.0012 $[m^3]$
SCR Volume Open Portion	ζ_{SCR}	0.83 $[-]$
Surface Coverage Fraction	θ_{NH_3}	0.35 $[-]$
Universal Gas Constant	R	8.3145 $[J/mol\ K]$

tunables parameters (frequency factors k_i and activation energy factors E_i) after the application of DoE.

The 0D model was checked for a different steady state conditions and different ammonia injections, then compared with signals provided by exhaust measurement systems. Figures 3 and 4 shows the comparison between the signal provided by Fourier-Transform Infrared Spectroscopy (FTIR) gas analyzer and by 0D model.

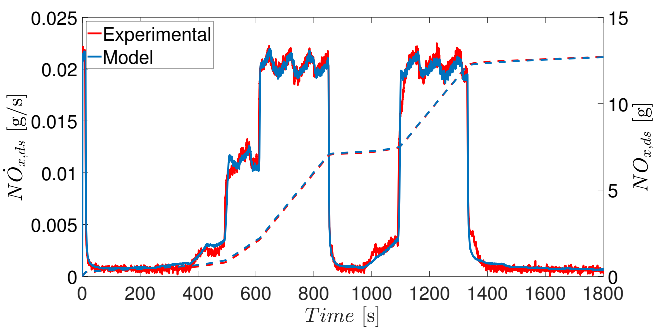

Figure 3. Comparison between FTIR and 0D model for NO_x downstream. Continuous line (——) is the instantaneous value (left axis) and the dashed line (- - -) is the cumulative value (right axis).

As can be seen, the measured and modeled signals (both instantaneous and accumulated) show a good agreement, specially in terms of NO_x (Figure 3). The highest differences can be appreciated in the NH_3 slip (Figure 4).

The higher model error in terms of NH_3 than in terms of NO_x can be justified by two main reasons: On the one hand, the NH_3 slip is more sensitive to the catalyst NH_3 load than NO_x, so potential errors in the estimation of amount of NH_3 stored in the SCR catalyst are transmitted to the NH_3 slip. On the other hand, the model is aimed to minimise ammonia injection with constraints on NO_x slip, so the identification

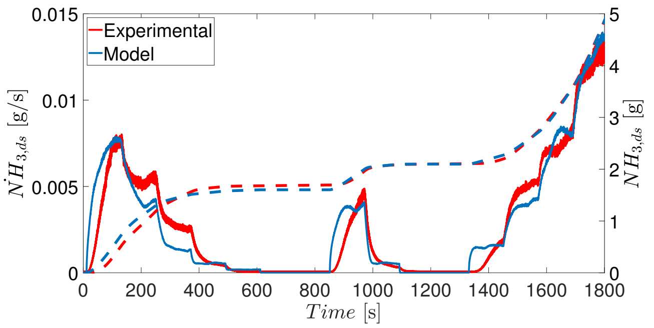

Figure 4. Comparison between FTIR and 0D model for NH_3 downstream. Continuous line (——) is the instantaneous value (left axis) and the dashed line (- - -) is the cumulative value (right axis).

efforts have been mainly focused in minimising the error in terms of NO_x.

Regarding validation, Figures 5 and 6 show the SCR model results when applied to the WLTC cycle.

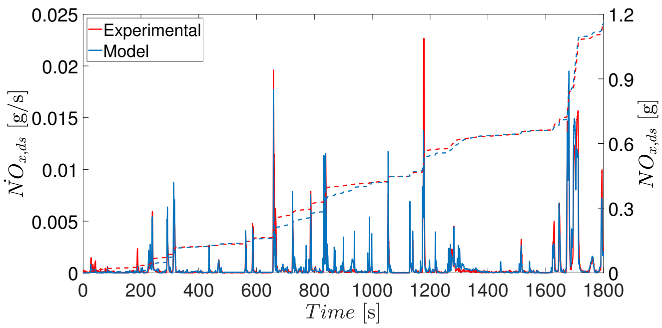

Figure 5. Comparison between FTIR and 0D model for NO_x downstream in a WLTC cycle. Continuous line (——) is the instantaneous value (left axis) and the dashed line (- - -) is the cumulative value (right axis).

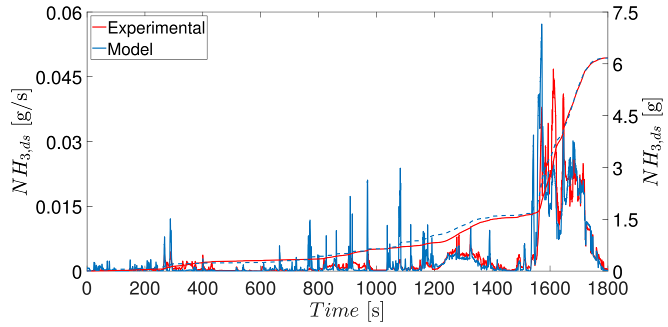

Figure 6. Comparison between FTIR and 0D model for NH_3 downstream in a WLTC cycle. Continuous line (——) is the instantaneous value (left axis) and the dashed line (- - -) is the cumulative value (right axis).

For NO_x signal differences can be appreciated at very high concentrations, when the evolution of NO_x downstream change quickly. Using 0D models, then without spatial discretisation usually lead to this kind of limitations since the transport of species between two sections is not properly captured. In any case, the correlation between measurement and model signals for the total amount of NO_x downstream concentration can be considered enough for the study purposes, reaching a 99.7%

As expected, higher differences can be appreciated in the NH_3 signal. In the NH_3, the detachment between the two signals can be attributed to boundary conditions of the model, since the adsorption and desorption of ammonia depend on the exact amount stored in the SCR, and these variables are difficult to control in an experimental dynamic test. The correlation between measurement and model signals for the total amount of NH_3 downstream concentration was 99.3%

In conclusion, as in constant engine parameters, the model is able to capture to a substantial extent the NO_x and NH_3 trends. In this sense, the model has been considered accurate enough for the optimization study.

Optimization tool

The problem addressed in the present paper, i.e. find the optimal ammonia injection that minimises its consumption in a given driving cycle with NO_x emissions constraints, matches perfectly with the OC theory. In particular the problem can be mathematically formulated as:

$$min_u \left\{ \int_0^{\tau} \dot{m}_{NH_{3,injected}}(u, x, w)dt \right\} \tag{11}$$

where u is the control variables, x is the vector of state variables (states of the SCR model described in Eqs. 6-10 and w is the vector of disturbance variables (flow, temperature and concentrations at SCR inlet):

$u = NH_{3,injection}$
$x = NO_{ds}; \quad NO_{2,ds}; \quad NH_{3,ds}; \quad \theta_{NH_3}$
$w = \dot{m}_{exh}; \quad T_{SCR}; \quad NO_{us}; \quad NO_{2,us}$

The limitations in the SCR and injection system can be included in the optimization problem as constraints in the states and controls:

$$min[x \quad u] \leqslant [x \quad u] \leqslant max[x \quad u] \tag{12}$$

The NO_x emissions limit can be included in the OC formulation as an integral constraint:

$$\int_0^{\tau} \dot{m}_{NO_{x,ds}}(u, x, w)dt < \bar{m}_{NO_{x,ds}} \tag{13}$$

where $\bar{m}_{NO_{x,ds}}$ is NO_x emission limit.

Regarding the optimization algorithm employed, the OC problem previously described has four states (NO_{ds}, $NO_{2,ds}$, $NH_{3,ds}$, and θ_{NH_3}) and a single control action ($NH_{3,injection}$). The model complexity and the relatively high number of states (4) suggests the use of a Direct Method (DM) implementation instead other alternatives such as Dynamic Programming or Potryagin's Minimum Principle. The DM is a family of optimal control methods that are based on transcribing an Optimal Control Problem (OCP) into a large but sparse non-linear programming problem. The last is much easier to solve and there are commercial and freeware NLP solvers that make use of advanced and efficient state-of-the-art algorithms to find an optimal solution[43]. Amongst the different methods to transcribe a continuous OCP into a finite NLP, Euler's collocation method is used since it is a first order numerical method and thus only two terms are needed to approximate an ordinary differential equation (ODE) then contributing to the sparsity of the problem matrix. Figure 7 shows the Jacobian matrix of the addressed OC problem, it can be observed that despite it is considerably large (201829x252284), only few elements are non-zero, in particular a 0.0021% of the matrix elements.

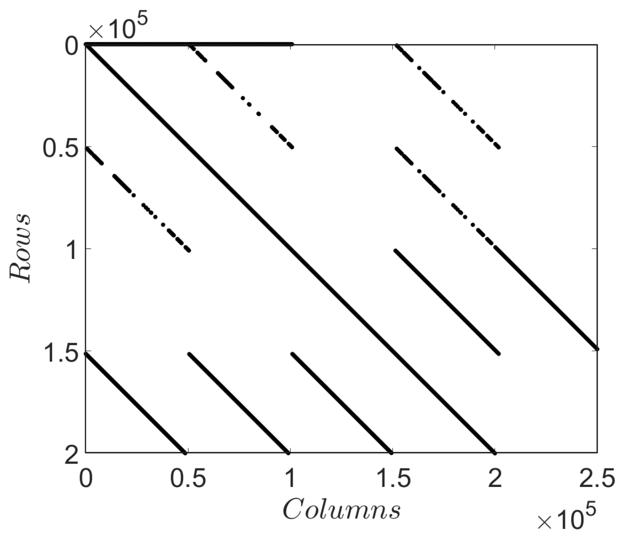

Figure 7. Jacobian matrix of the transcribed NLP. Black dots are non-zero elements.

Further details in the DM algorithm employed can be found in Reig[44]. Regarding the NLP solver used, in this work IPOPT[43], an open source solver, has been used.

Results and discussion

In this section, the results obtained with the optimization tool are shown.

Model results

This subsection presents the comparison between the model output signal and the measured experimental data.

With the optimization tool working properly, the WLTC cycle with different NO_x downstream limits was optimized. In Figure 8, x-axis is the amount of NO_x downstream and y-axis is the amount of ammonia injected in a WLTC cycle. Figure 8 shows the pareto front obtained from the model optimization and the red star (point 'A') representing the experimental results with standard calibration.

One can identify two cases of particular interest: The strategy 'B' that minimises the ammonia consumption to keep the NO_x emissions in the same level than the standard strategy (iso NO_x), and the strategy 'C' that is aimed to minimise the NO_x emissions with the same ammonia consumption than the standard strategy (iso NH_3). For iso NH_3 the NO_x downstream is reduced by 14.1%, and for iso NO_x a 33.5% of the ammonia consumption was saved.

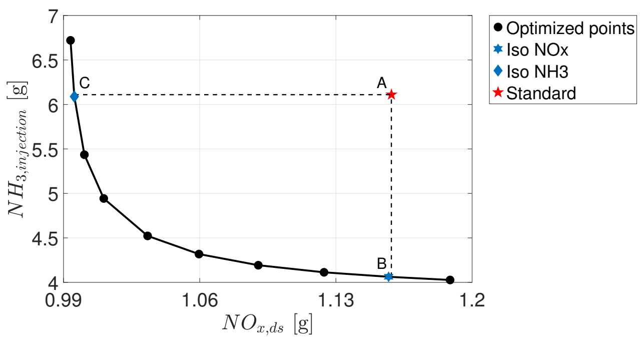

Figure 8. Comparison between optimization model and standard calibration for total amount of NO_x downstream and NH_3 injected in a WLTC cycle.

Experimental results

The experimental validation of the previously described optimization is done by imposing the calculated ammonia injection policies in the test bench during a WLTC.

Figure 9 shows the comparison of the experimental results obtained with the standard strategy and the iso NH_3 optimized strategy. Two main differences between the standard and optimized strategy can be observed. On the one hand, the standard strategy provides a smoother evolution in the injection while the optimized strategy shows frequent jumps between relatively no injecting and inject relatively high levels of ammonia. On the other hand, one can observe that in order to minimise the NO_x emissions with a given amount of ammonia injected, it is more efficient to increase the ammonia injection at the beginning of the cycle to keep the SCR with a high load, and therefore high NO_x efficiency, during the complete cycle. The increase in ammonia consumption during the first phases of the cycle can be compensated at the end of the cycle since the SCR dynamics will prevent the ammonia injected in this last phase of the cycle to have a substantial impact on the NO_x emissions in the cycle. This policy, jumping from high to low levels in the actuation and focusing the actuation in the first phases of the cycle is in line with the general solution of dynamic systems optimization that usually leads to maximum power at the early phases of the problem and coasting in the last phases. Some examples of similar policies applied to other powertrain optimization problems can be found in Guardiola *et al.* [45] which presents the optimal heat release shaping minimising the indicated specific fuel consumption in a reactivity controlled compression ignition (RCCI) engine, Maria Desantes *et al.* [46] shows the optimal depletion strategy of the three way catalytic converter for minimum fuel consumption, and Zhu *et al.* [47] shows the fuel-optimal speed profile in eco-driving strategy for parallel hybrid-electric vehicles using the artificial neural networks. Results also point out that NO_x can barely be further reduced from the iso NH_3 results since the ammonia load of the SCR is kept at near maximum levels during the complete cycle. This conclusion can be also observed in Figure 8 where NO_x approaches asymptotically to 0.99 g at the expense of noticeably increases in ammonia injection.

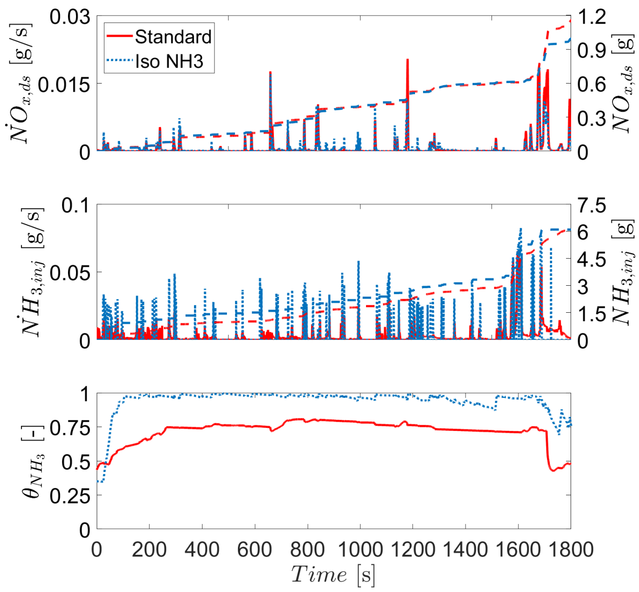

Figure 9. Comparison between experimental results obtained with the standard calibration and the iso NH_3 optimal strategy for NO_x emissions (upper plot), NH_3 injected (medium plot) and SCR ammonia loading (θ_{NH_3}) in the WLTC. Continuous line (——) is the instantaneous value of the Standard calibration, dotted line (⋯⋯) is the instantaneous value of Iso NH_3 and the dashed line (- - -) is the cumulative value (right axis).

Analogously, Figure 10 shows the comparison of the experimental results obtained with the standard SCR control and the NO_x optimized strategy. Results show how the efficiency of the ammonia injection can be improved to keep the same NO_x emissions that the standard strategy with a substantial saving in ammonia consumption. Again, results point out that a switching strategy between high and low ammonia injections is more efficient than introducing ammonia in a smoother way. However, in this case, the required efficiency in the SCR is not as high as in the case of iso NH_3 strategy, so the NH_3 storing level is kept at medium values.

The experimental ammonia consumption and NO_x emissions of the different tests carried out are shown together with the modelling results in Figure 11. The model and

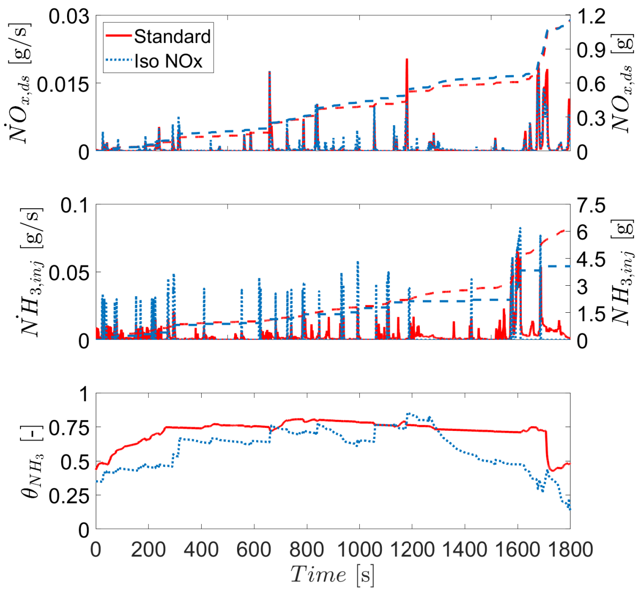

Figure 10. Comparison between experimental results obtained with the standard calibration and the iso NO_x optimal strategy for NO_x emissions (upper plot), NH_3 injected (medium plot) and SCR ammonia loading (θ_{NH_3}) in the WLTC.Continuous line (——) is the instantaneous value of the Standard calibration, dotted line (······) is the instantaneous value of Iso NO_x and the dashed line (- - -) is the cumulative value (right axis).

experimental results show a high correlation then validating the OC approach as a method to optimize the ammonia injection in a predefined driving cycle.

As can be seen in Figure 11, an experimental test was carried out at another point in the optimization strategy (Opt D). This test aimed to verify the model in a condition of simultaneous optimization, where the improvement is in terms of ammonia consumption and NO_x emissions.

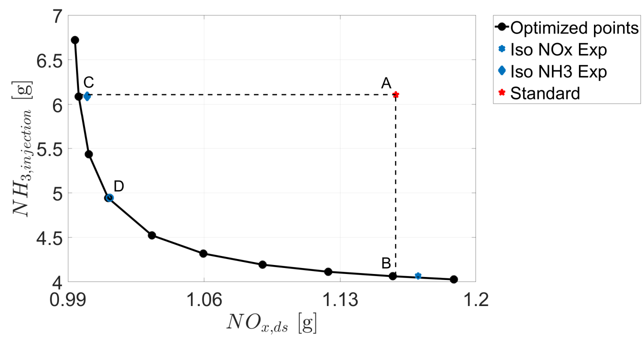

Figure 11. Comparison between optimization model and experimental results for total amount of NO_x downstream and NH_3 injected in a WLTC cycle.

Table 5 shows the results of the amount of ammonia injected and NO_x downstream with standard and optimized (simulated and experimental) ammonia injection strategy. With the experimental results, for Iso NO_x was saved 33.5% of ammonia consumption, for iso NH_3 was reduced NO_x downstream by 13.7% and for the condition of simultaneous optimization (Opt D), a reduction of 19.1% in ammonia consumption and 12.7% in NO_x emissions.

Table 5. Results

Strategy	NH_3 [g]	NO_x [g]	
		Simulated	Experimental
Standard	6.110	1.159	1.159
Iso NH_3	6.092 [0.29%]	0.996 [14.1%]	1.000 [13.7%]
Iso NO_x	4.063 [33.5%]	1.157 [0.17%]	1.170 [-0.95%]
Opt D	4.943 [19.1%]	1.011 [12.8%]	1.012 [12.7%]

The results obtained place the standard control strategy of the SCR in the plane of ammonia consumption and NO_x emissions of the vehicle allowing its evaluation. Eventually, the previous procedure can be done with a different SCR design and the comparison of the obtained pareto fronts will rank them according to its potential performance. In addition, the analysis of the optimized strategies gives insight on the design of realtime control strategies, in the case at hand, it is more efficient to use more aggressive ammonia injection strategies, with frequent changes in the ammonia injection level between low and high values than using a smooth ammonia evaluation. In the same line, the comparison of ammonia load in the SCR of iso NO_x and iso NH_3 strategies allows to observe a correlation between the average ammonia load and the final NO_x emissions. Accordingly, a model-based control strategy aimed to keep the ammonia loading of the SCR seems a feasible approach for realtime SCR control with near-optimal results.

Finally, it should be noted that the OC approach allows to include other constraints in the problem such as NH_3 slip, maximum or minimum SCR temperatures or, in general, any variable that can be obtained from the model states, disturbances and actuators.

Conclusions

The paper has explored the use of Optimal Control to obtain the optimal ammonia injection strategy, in the sense of minimum ammonia consumption with constraints in NO_x emissions during the WLTC. The experimental results obtained show that a state of the art 0D control oriented model has the required accuracy to represent the main phenomena in the SCR to provide realistic estimations while keeping simplicity to be embedded in a Direct Method optimization without prohibitive computation cost. In this sense, it has been proven that Optimal Control is a valuable tool for SCR design (including its control strategy) since the obtention of the pareto front allows to benchmark different design alternatives. The main specific contributions of this work are:

- State of the art control oriented models of the SCR are able to represent with a substantial degree of accuracy the behavior of the SCR catalyst, with low computation burden so can be integrated in optimization tools.
- The evaluation of a state of the art SCR control strategy show that optimization can lead to a 33.5% of ammonia saved while keeping the same NO_x emissions or conversely, NO_x can be reduced in a 13.7% without ammonia increase. It is also possible to simultaneously improve ammonia consumption and NOx emissions.

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Nomenclature

Acronyms

NH_3	Ammonia
CSTR	Continuously Stirred Tank Reactor
DOC	Diesel Oxidation Catalyst
DPF	Diesel Particulate Filter
ECU	Electronic Control Unit
EGR	Exhaust Gas Recirculation
FTIR	Fourier-Transform Infrared Spectroscopy
ICE	Internal Combustion Engine
NO_x	Nitrogen oxides
NLP	Non-linear Programming
OBD	On-Board Diagnostics
OC	Optimal Control
OCP	Optimal Control Problem
ODE	Ordinary Differential Equation
RDE	Real Driving Emissions
SCR	Selective Catalytic Reduction
SCRF	Selective Catalytic Reduction System Filter
SV	Spatial Velocity
VGT	Variable Geometry Turbine
WLTC	Worldwide Harmonized Light Vehicles Test Cycle

Greek letters

θ	Storage on the catalyst surface $[-]$
α	Surface coverage $[-]$
δ	Gas density $[\mathrm{kg/m^3}]$
ζ	Open portion of the SCR volume $[-]$
Ω	SCR storage capacity $[\mathrm{mol/m^3}]$

Subscripts

a	Adsorption
d	Desorption
ds	Downstream
exh	Exhaust
inj	Injected
fst	Fast
ref	Reference
slw	Slow
std	Standard
us	Upstream