

New Methodology for Transient Engine Rig Experiments for Efficient Parameter Tuning

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ABSTRACT

When performing catalyst modeling and parameter tuning it is desirable that the experimental data contain both transient and stationary points and can be generated over a short period of time. Here a method of creating such concentration transients for a full scale engine rig system is presented. The paper describes a valuable approach for changing the composition of engine exhaust gas going to a DOC (or potentially any other device) by conditioning the exhaust gas with an additional upstream DOC and/or SCR. By controlling the urea injection and the DOC bypass a wide range of exhaust compositions, not possible by only controlling the engine, could be achieved. This will improve the possibilities for parameter estimation for the modeling of the DOC. Important features of the resulting data include fast transients in concentrations with only small variations in temperature, CO concentrations with HC concentrations close to zero, and NO concentrations close to zero with significant NO₂ concentration.

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INTRODUCTION

The diesel oxidation catalyst (DOC) is a well established technology to reduce CO and hydrocarbon (HC) emissions from diesel engines. Strengthened emission standards have made the importance of the DOC even greater in recent years since it plays an indispensable role in enhancing the performance of diesel particulate filters (DPF) and selective catalytic reduction (SCR) by enabling NO oxidation to NO₂ [1]. Therefore correct predictions of the DOC performance are very important for simulations of the entire aftertreatment system.

In order to perform successful parameter estimation for modeling, data properties, such as a large experimental space and decoupling of effects and variables are of utmost

importance. To achieve these properties of the data laboratory scale experiments are generally used for kinetic parameter estimation [2]. In laboratory scale it is possible to use essentially any combination of exhaust gas composition and temperature which makes it possible to estimate parameters over a wide range of conditions. This can be enabled by model-based design of experiments which explores the range of experimental conditions suitable for parameter estimation [3]. It is however difficult to fully replicate the properties of engine exhaust at lab scale. The hydrocarbon (HC) composition is for example very complex which means that a retuning of the parameters usually is necessary when kinetic parameters from lab scale are applied on a full scale system. The parameter retuning from full scale engine rig experiments such as demonstrated by Wang et al. [4], is

limited by the exhaust compositions that are possible for the engine to produce. For example in an engine exhaust, the concentration of CO is closely linked to the concentration of HC and the concentration of NO₂ is closely linked to the concentration of NO. When switching between two engine operating points it also generally takes several minutes before the properties of the emissions have stabilized. The main reason for this lag in response is the large thermal mass between the engine and the investigated catalyst which will not only affect the transient behavior of the temperature but also of the concentrations. This behavior not only makes the experiments time consuming, but it also complicates the transient modeling of the DOC since the changes in inlet properties are far from ideal step functions. These resulting, relatively slow transients in feed concentration which are also convoluted with feed temperature transients, may provide little direct information regarding the transient behavior of the catalyst, due to for example the adsorption/desorption of reacting species and changes in the pool of adsorbed intermediate species.

Kolaczkowski et al. [5] presented a method where a pollutant (e.g. CO or propane) was injected between the engine and the studied DOC to achieve transient data without changing the engine operating point. This method also offers the great benefit that the heat accumulation problem is avoided, since the engine operating point and thereby the temperature is constant, and thus very fast transients in concentrations can be achieved. Sjöblom [6] further extended this concept by also having the possibility to reduce the flow (increase residence time) and control the temperature. The reaction rates are highly dependent on both exhaust composition and temperature and the possibility to change these variables independently will significantly improve the conditions for parameter estimation.

The current study presents an approach where additional catalysts are used to change the inlet concentrations to the test-object (DOC). Since the transients are induced only by switching valve positions and SCR-control, instead of variation of engine operating point, experimentation with quicker and more selective variation in inlet conditions is enabled. Inlet compositions far from what is possible with only an engine can be achieved which will aid the estimation of parameters. In the current study the experimental setup is described and a few illustrative examples are given to describe the typical results from this concept.

EXPERIMENTAL SECTION

To achieve more controlled and faster changes in the inlet emission concentrations to the catalyst an extra DOC with the possibility for bypass flow and an SCR with urea injection were mounted before the catalyst, as illustrated in [figure 1](#).

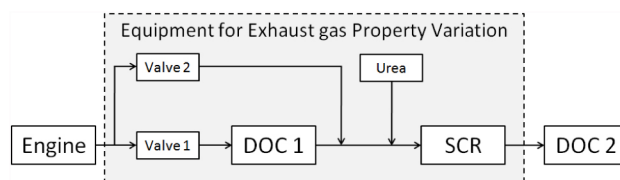


Figure 1. Experimental set-up. “DOC 2” is the test-object to be studied

The fraction of exhaust gas flow through DOC 1 allowed variation in the conversion of HC and CO to CO₂ and H₂O, and the conversion of NO to NO₂. By injecting different amounts of urea the conversion of NO₂ and NO to N₂ was controlled and the ratio of NO₂ to NO_x could be adjusted. The engine was also tuned to run with late fuel injection to achieve high HC and CO concentrations. A Vanadium-based commercial full-size SCR and a commercial platinum-only full-size DOC was used for exhaust gas property variation.

A Scania heavy duty diesel engine was used as the exhaust source and Swedish MK1 diesel, a commercial low-sulfur (approximately 5 ppm S) diesel, was used as fuel. The engine was equipped with a dynamometer control system enabling independent control of load and speed.

The experimental set-up was used for three different types of experiments that will be described in detail below. All experiments were run at more than 20 different engine operating points which resulted in a wide range of transient inlet conditions to the test-objects (DOC 2 in [figure 1](#)). Parameter tuning on the test-objects, which consisted of several different catalyst configurations, will be performed in a future study. To highlight the comparison between the experiment types the results for only one single operating point will be reported here. The operating point selected was at medium exhaust temperature (ca 300 °C), high flow rate (ca 0.3 kg/s) and medium concentrations of NO, NO₂, CO and HC. It should be noted that the N₂O levels measured from the SCR were below 2 ppm for the presented data and will therefore not be included in the figures.

RESULTS AND DISCUSSION

Three different types of experiments were run with the set-up introduced in [figure 1](#). These will be referred to as type 1, 2 and, 3 experiments and will be thoroughly described in the following sections. The experiments types differ in the manner in which the transients are generated. In experiment type 1 the transients were created by changing the by-pass valve position, in experiment type 2 by changing the urea injection, and in type 3 by changing the by-pass valve position as well as the urea injection.

In the presentation of the results the thermodynamic equilibrium for the NO oxidation reaction will be frequently used as a reference (noted as “NO at eq.” and “NO₂ at eq.” in the figures). These limits are calculated from the inlet concentrations of NO, NO₂, and O₂ and the inlet temperature

to the test-object. The purpose is mainly to show the limits for the conversion of NO to NO₂ in the DOC, but also to show how the NO_x reduction in the SCR affects these limits.

Type 1 Experiments - DOC Bypassing with No SCR

In this first experimental set-up the urea injection and SCR were eliminated from the configuration shown in [figure 1](#) to create a system with simpler dynamic behavior closer to ideal steps and where a high inlet concentration of HC to DOC 2 was possible. By switching valve 1 position between 20% and 90% open at the same time as valve 2 was switching between 80% and 10% open, fast transients in inlet concentrations to DOC 2 of CO, HC and NO_x were achieved (see [figure 2](#)). The difference in maximum and minimum valve positions for valve 1 and 2 were selected to compensate for differences in flow resistance between the two pathways. The selected positions resulted in about the same maximum and minimum flows through both pathways. [Figure 2](#) also shows small variations in temperature between 302°C and 304°C which mainly originate from a difference in heat loss between the bypass pipe and DOC 1.

The graphs of NO oxidation thermodynamic equilibrium in [figure 2](#) show how DOC 1 pushed the concentrations of NO and NO₂ closer to what is thermodynamically possible for the NO oxidation reaction. The figure also shows that the concentration of NO₂ could exceed the NO concentration for an extended period of time at these conditions and that the concentrations reached stable values in a few seconds. Neither of these properties would be achievable by only changing the engine load point.

Type 2 Experiments - Fixed DOC Bypassing with Urea SCR

In this type of experiment the set-up was according to [figure 1](#) and the purpose was mainly to widen the possible NO₂/NO_x relation and NO_x dynamics compared to experiments of type 1. The valve positions were locked at specific positions and urea was injected in pulses of 20 seconds. Five different combinations of flow through bypass and DOC 1 were used for the selected engine operating point according to [table 1](#). In [table 1](#), configuration 1 gives highest NO₂/NO_x ratio to the SCR and configuration 5 gives the lowest NO₂/NO_x ratio.

Table 1. Bypass configurations for experiment type 2, valve positions in % open

Configu- ration	1	2	3	4	5
Valve 1 position	100%	67%	50%	33%	0%
Valve 2 position	0%	33%	50%	67%	100%

In [figure 3](#) the results from an experiment of type 2 with bypass configuration 1 (see [table 1](#)) and the same engine operating point as in the previously described experiment are shown. The reason for selecting configuration 1 here is that this leads to the NO₂/NO_x ratio in the SCR inlet closest to the optimal ratio of 0.5 and thus the highest NO_x reduction in the SCR. Note that this is not necessarily the case for other engine operating points.

For the selected valve position configuration and engine operating point virtually all HC and CO were reduced in DOC 1 and since no valve positions were changed during the experiment the experimental data is sufficiently described with only the two panels in [figure 3](#).

Two cycles with successively increasing urea dosage (0%, 30%, 60% and 90% of stoichiometric NO_x reduction) were performed, where the measured urea dosage can be seen in [figure 3](#). The figure also shows some important features of the experiment type where the most noticeable one is that the NO₂ concentration was higher than the NO concentration throughout the experiment. The reason is, of course, that all flow was through DOC 1 for this configuration (1) where NO was oxidized to NO₂. In other words, the different configurations in [table 1](#) had a large influence on both the NO₂/NO_x ratio, and the CO and HC concentrations in the SCR inlet and the results in [figure 3](#) represents only one of the most extreme cases.

At the highest urea injection, the rare case was achieved where the NO concentration was close to zero while the NO₂ concentration was as high as 100 ppm. At the same time both the NO and NO₂ concentrations were approaching values close to the thermodynamic limits for the NO oxidation reaction. Theoretically the SCR reactions make it possible to even exceed these thermodynamic limits, which was also measured in some experiments, however only very briefly. The NO_x fluctuations, which can be seen in [figure 3](#), were a result of pressure pulses applied to remove urea stored in the injection system due to imperfect mixing between urea and injected pressurized air. The urea removed with these pressure pulses reacted with NO_x resulting in sharp dips in both NO and NO₂ that could even occur when no urea was injected.

Type 3 Experiments - DOC Bypassing with Urea SCR

The third type of experiment was a combination of the first two types, intended to provide an even wider variation in composition to the test-object. The set-up was the same as for type 2 experiments but to achieve even more dynamic concentration changes the valve positions were no longer locked; instead they were changing every 20 s in the same way as in type 1 experiments. With the purpose of making the data even more information rich urea was injected, for at least 20 s, with a 10 s delay relative to the changes in valve position. The position of the valve 1 relative to the urea

injection set-point is shown in panel b) of [figure 4](#). The results from one experiment of type 3, at the same engine operating point as experiment type 1 and 2 previously shown in [figures 2](#) and [3](#), are shown in [figure 4](#).

[Figure 4](#) shows that the CO and HC concentrations were unaffected by the variations in urea dosage. This is expected since the formed ammonia will mainly react as a NO_x reductant and take part in undesired side reactions involving oxygen [7]. When [figure 4](#) is compared to [figure 2](#) it is also evident that the SCR catalyst itself reduced the concentration of HC considerably but had only a small influence on the CO concentration, which was slightly increased. At engine operating points with higher temperatures than the one used in [figure 4](#), all the HC was consumed in this manner which gave high CO concentrations in the inlet to DOC 2 but no HC. This is difficult to achieve in exhaust from a standard engine rig where only the engine operating point can be changed since HC and CO concentrations generally are strongly coupled. [Figure 4](#) also shows the urea dosage set-point corresponding to 0%, 30%, 60% and 90% of the stoichiometric NO_x reduction.

[Figure 4](#) shows that the temperature fluctuations were small for this experiment, although a small increase of up to 4°C can be seen between 300 and 500 seconds where the NO_x was reduced continuously for a longer period of time. The NO concentration was influenced strongly by both the urea dosage and the flow through the DOC 1.

Table 2. Description of the inlet conditions resulting from the changes in urea dosage and bypass of DOC 1 during the 40 seconds cycles in the first part of the experiment type 3.

Inlet conditions	Urea dosage	Valve 1 position	Valve 2 position	Description
1	Off	90 %	10 %	NO ₂ /NO _x ≈ 0.5 since main flow through DOC 1
2	Off	20 %	80 %	Low NO ₂ since main flow through by-pass, high NO since no urea injected
3	On	20 %	80 %	NO only consumed via standard SCR reaction [8] since NO ₂ concentration is low, only small amount of NO reduced by ammonia
4	On	90 %	10 %	Higher NO ₂ /NO _x ratio gives more reduction of both NO and NO ₂ via fast SCR reaction [8]. All NO ₂ reduced by ammonia.

The delay between the urea dosage and bypass of DOC 1 resulted in different inlet conditions to the test-object during 40 second cycles in the first part of the experiment (up to about 290 s). The different inlet conditions during one such cycle are described in [table 2](#) together with the urea dosage and valve positions.

In [figure 5](#) the results of one cycle, as described in [table 2](#), are depicted for measurement data between 134 and 184 s (from [figure 4](#)). Condition 1 can be identified at 134-148 s, condition 2 at 148-155s, condition 3 at 155-168 s and condition 4 at 168- 176 s. The transition from one condition to another is, however, not clear cut, which mainly is a result of the deviation between urea set-point and urea dosage. As an example, inlet condition 3 where urea dosage is on and the position of valve 1 is 20 % open only lasted for about 5 seconds (161 s to 166 s). The real inlet conditions to the test-object will in other words be in transition between the inlet conditions described in [table 2](#) for the majority of the cycle time.

If the NO₂ concentration for the first 300 s of the experiment ([figure 4](#)) is studied it can be noted that the first two peaks (starting at around 40 s and at around 80 s) broke through even when the urea injection was still at its highest value. The reason for the 100% NO₂ reduction before the peak broke through must therefore be that ammonia injected at an earlier time point where the NO₂/NO_x ratio was low (due to a high bypass flow) was stored and therefore was available for fast SCR reaction when the NO₂/NO_x ratio was increased. When the urea dosage was increased, the NO₂ broke through increasingly later after the urea injection was stopped, resulting in increasingly narrower NO₂ peaks which also indicates an increased storage.

Between 300 and 580 s in [Figure 4](#), it can also be seen that the highest urea dosage was enough to reduce all NO₂ but for the lower dosages some NO₂ reached the test-object when the main flow was through DOC 1 resulting in peaks at 310, 350 and 400 s. At about 485 s the concentration of HC briefly exceeded the concentration of NO_x. Again, this is not achievable in a standard engine rig exhaust but was made possible here when the NO₂/NO_x fraction was close to 0.5 in the SCR inlet (since the main flow was through DOC 1) at the same time as the urea injection was high. The reason that not all HC was reduced in DOC 1 and the SCR is due firstly to the moderate temperature and secondly to the high HC concentration in the engine exhaust as a result of the late fuel injection tuning of the engine.

CONCLUSIONS

The most apparent advantage with the demonstrated experimental set-up is the possibility to achieve fast transients in concentration with only small variations in temperature. Moreover the experimental data has also shown that the following engine rig exhaust gas features are enabled by the

experimental set-up that would not be possible with a standard engine rig:

- High CO concentrations with HC concentrations close to zero
- HC concentrations exceeding NO_x concentration
- NO concentrations close to zero with significant NO₂ concentration

The different experiment types presented also show the possibility to generate measurement data of varying complexity with the presented set-up.

The reduced correlation between temperature and concentrations, but also between individual concentrations of reactants, significantly widens the possible experimental conditions to aid full scale catalyst modeling and parameter tuning.

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ABBREVIATIONS

DOC - Diesel Oxidation Catalyst

HC - Hydrocarbons

SCR - Selective Catalytic Reduction

FIGURES 7 INCH

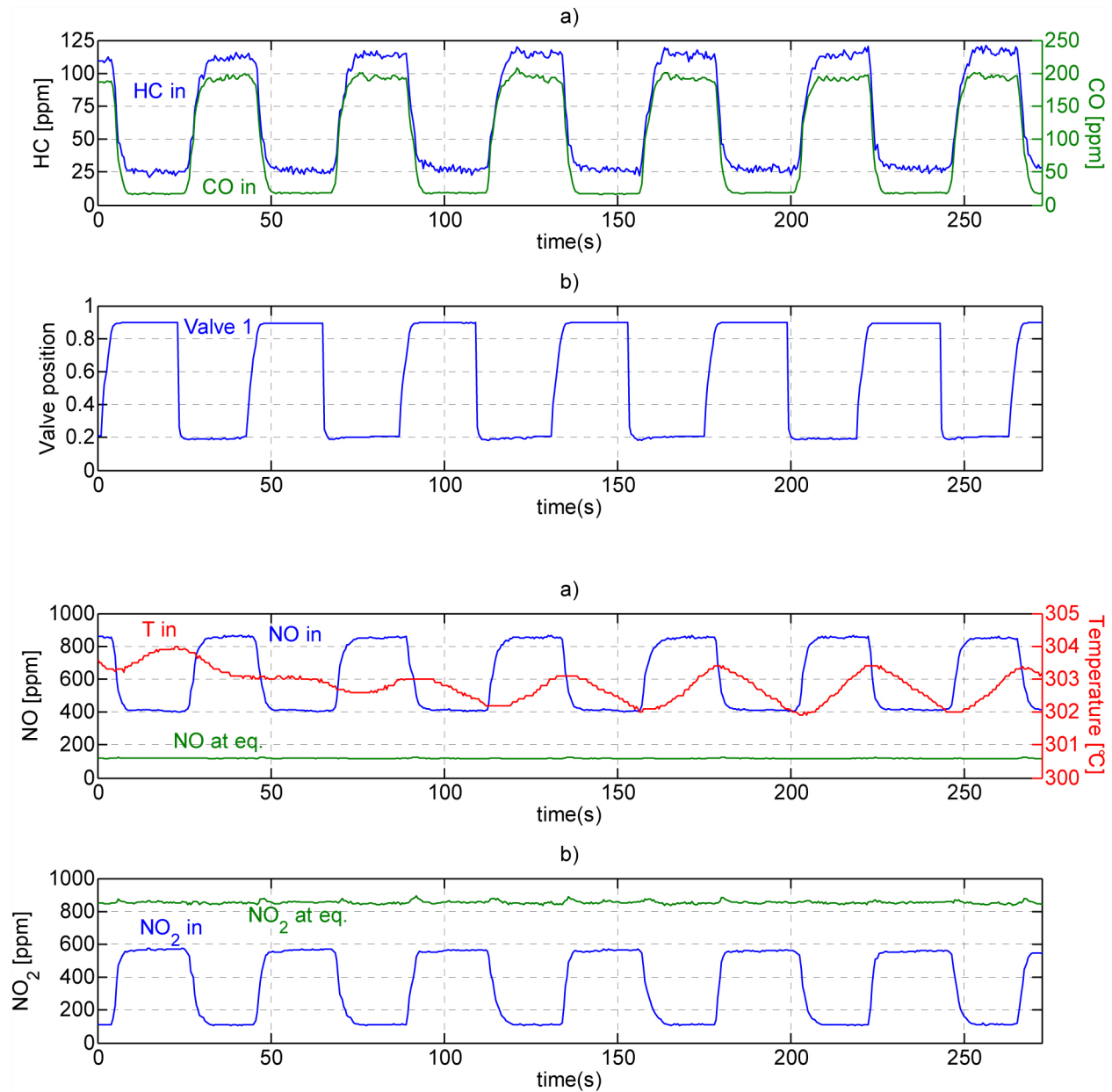


Figure 2. Data from experiment type 1. a) DOC 2 inlet mole fractions of CO and HC. b) valve position for valve 1 (see figure 1) where 1 is fully open and 0 is closed. c) DOC 2 inlet mole fractions and thermodynamic equilibrium for NO, and temperature. d) DOC 2 inlet mole fractions and thermodynamic equilibrium for NO₂

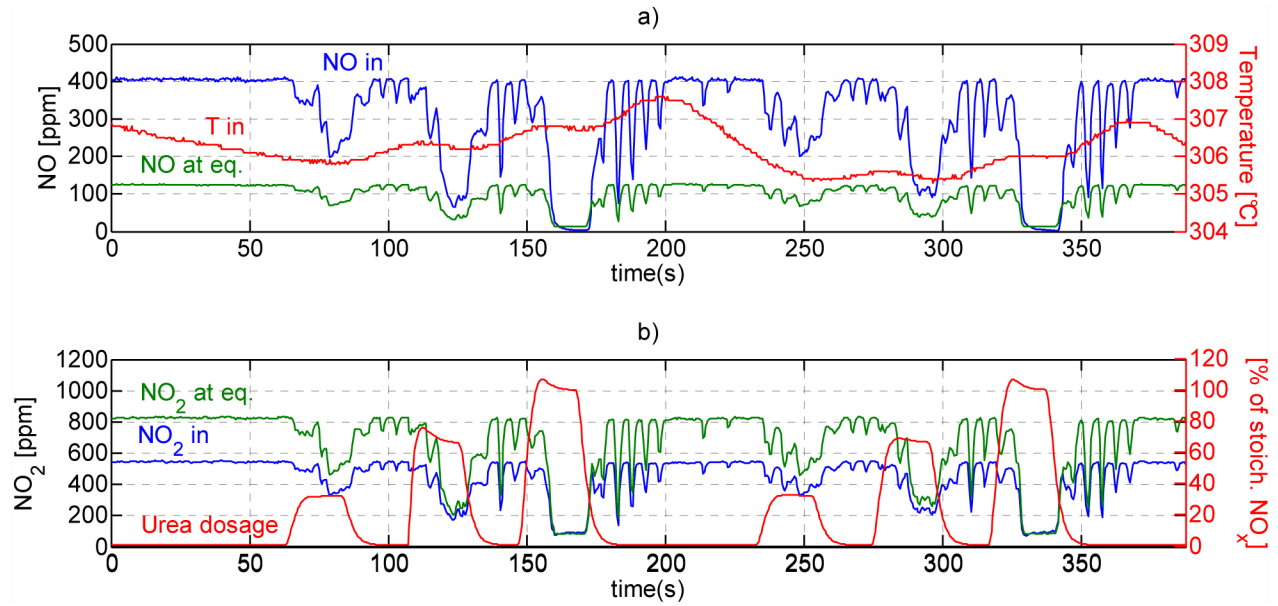


Figure 3. Data from experiment type 2. a) DOC 2 inlet mole fractions and thermodynamic equilibrium for NO, and temperature. b) DOC 2 inlet mole fractions and thermodynamic equilibrium for NO₂, and urea dosage

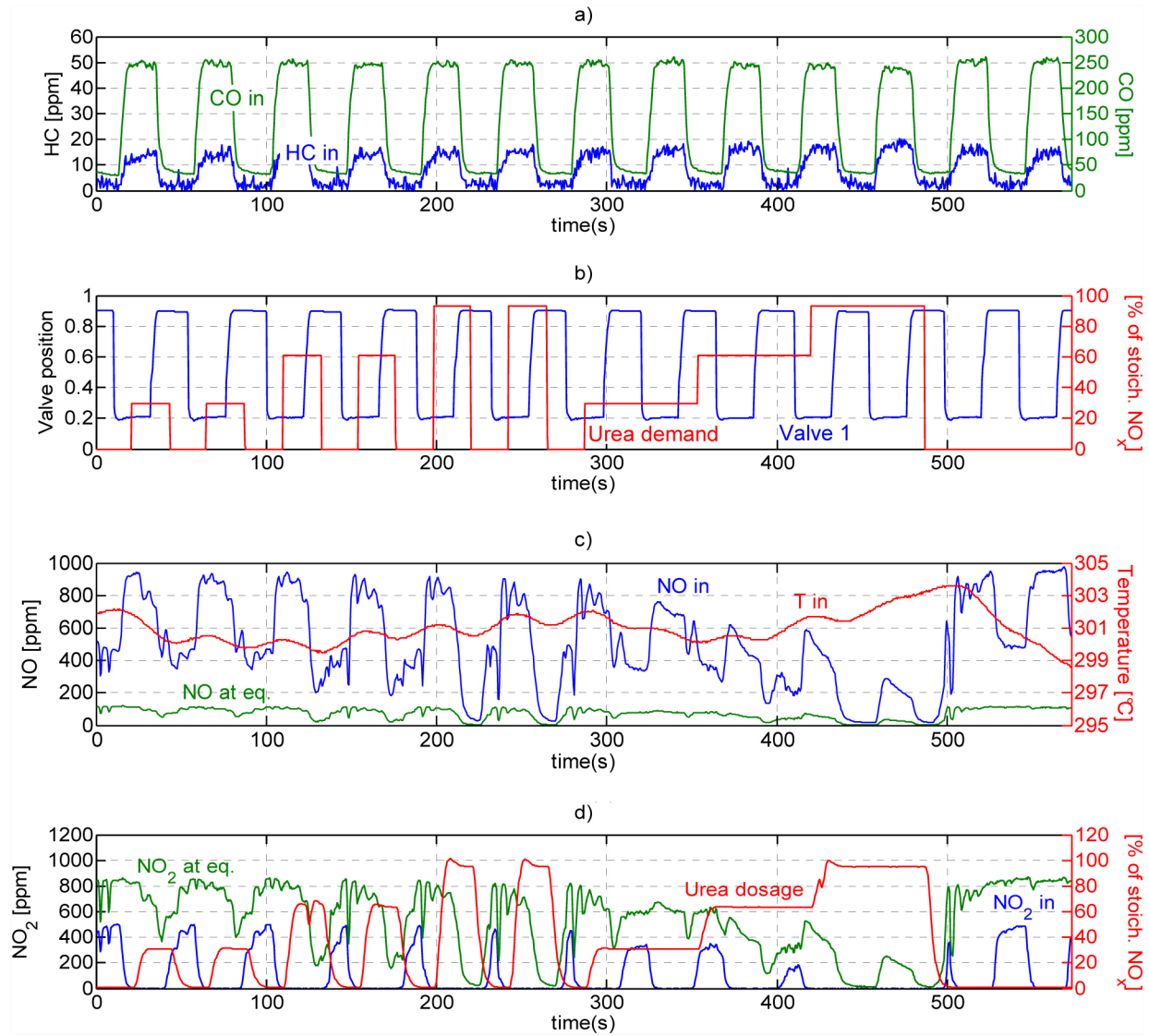


Figure 4. Data from experiment type 3. a) DOC 2 inlet mole fractions of CO and HC. b) valve position for valve 1 (see figure 1) where 1 is fully open and 0 is closed, and urea demand. c) DOC 2 inlet mole fractions and thermodynamic equilibrium for NO, and temperature. d) DOC 2 inlet mole fractions and thermodynamic equilibrium for NO₂, and urea dosage

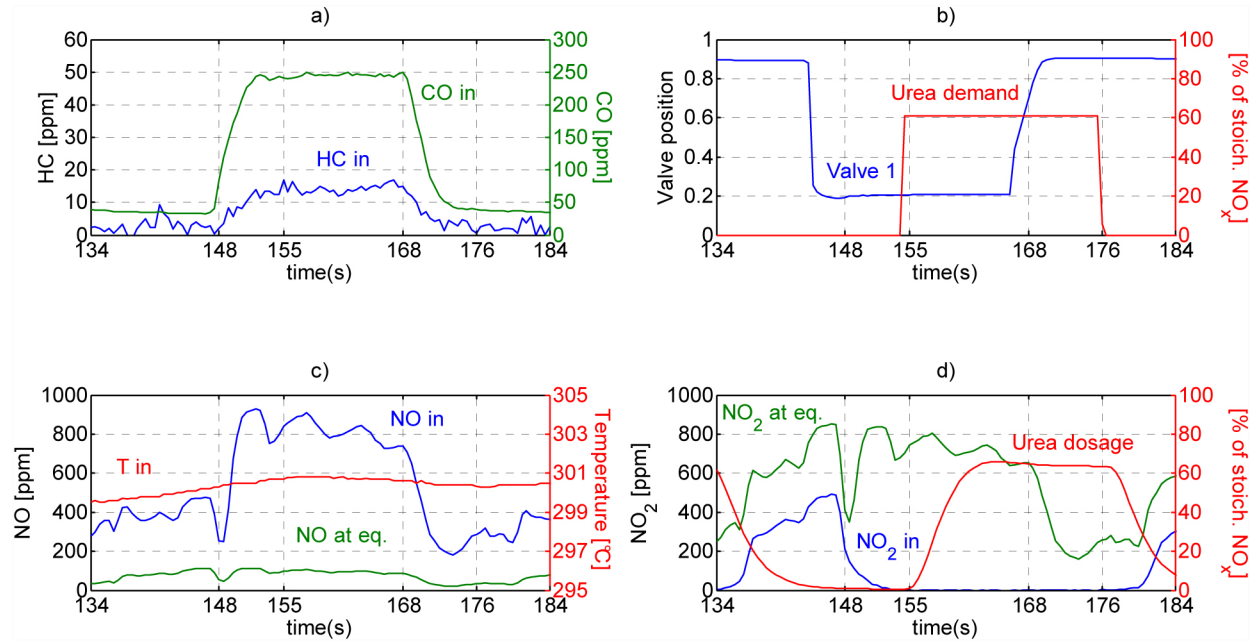


Figure 5. Magnification of the measurement data between 134 and 184 s from [figure 4](#) to show the conditions described in [table 2](#). a) DOC 2 inlet mole fractions of CO and HC. b) valve position for valve 1 (see [figure 1](#)) where 1 is fully open and 0 is closed, and urea demand. c) DOC 2 inlet mole fractions and thermodynamic equilibrium for NO, and temperature. d) DOC 2 inlet mole fractions and thermodynamic equilibrium for NO₂, and urea dosage