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Modelling of NO_x Conversion in a 1D Diesel Engine Exhaust SCR Catalyst System under Transient Conditions Using Ammonia Gas as the Reductant

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ABSTRACT

Use of selective catalytic reduction technology is the most popular strategy for removing NO_x from lean diesel exhaust. The reductant is essentially ammonia and this has been supplied as a spray of urea droplets, but more recently alternative technology where ammonia gas is released from a storage-medium has become a viable alternative. Experiments have been carried out on an engine test rig run to steady state conditions using NO_x composed of either 25 % or 50 % of NO₂, with ammonia gas as the reductant. This was a 1D study where a long 10 degree diffuser provided uniform temperature and velocity profiles to the SCR catalyst brick. Under the transient conditions that occur during drive cycles, the dosing of the ammonia can deviate from the optimum. In this study, the dosage rate of ammonia was held at a fixed value, while the engine load was varied. The variation was from low load to high load and back down for various time periods, based on the rates of change that are typical of those in engine drive cycles. A study where the change was from low load to high load but then remained high was also performed, and also where the change was from high load to low. The low engine load supply temperature was about 215°C, rising towards 300°C under steady state conditions at high load. The NO and NO₂ levels downstream of the SCR were measured using fast response CLD NO_x analysers in some of the experiments. The latter are sensitive to cross talk from ammonia so ammonia was under-dosed in those experiments and there was negligible ammonia slip downstream of the SCR where the CLD measurements were taken. In other experiments an FTIR analyser was used and higher ammonia dosing levels were investigated. The transients observed have been modelled in a CFD model using modified standard SCR reaction kinetics in a full kinetic scheme obtained from the literature. In the cases

where the % of NO₂ was about 25 it was necessary to enhance the slow SCR reaction rate to simulate the observations, but in the cases where the % of NO₂ was about 50 the fast SCR reaction dominated and gave a reasonable description of the observations. The model's ability to simulate transients in an SCR engine exhaust system is assessed in this paper.

INTRODUCTION

Passenger cars powered by Diesel fuel have their part to play in minimizing CO₂ emissions because they are lean-burn and fuel efficient but they are emitters of relatively high levels of NO_x. This is currently dealt with through innovative after-treatment systems combined with engine strategies. One such after-treatment system is Selective Catalytic Reduction. This requires a reductant to be introduced into the exhaust stream. The reductant is often ammonia and this is obtained either from the breakdown of droplets from an aqueous urea spray or directly by its release from a storage medium. The NO_x is reduced by the ammonia on an SCR catalyst. Regulating the supply of ammonia so that there is sufficient for the reduction but there is no ammonia slip from the exhaust system is paramount. The amount of ammonia that is required is approximately one mol of ammonia per mol of NO_x, as the so-called standard, fast and N₂O formation reactions proceed with this stoichiometry. The so-called slow SCR reaction, however, requires 4 mol of ammonia per 3 mol of NO₂ so the balance of NO_x consumed to ammonia consumed varies depending on the conditions prevailing during the transient, notably the temperature and the NO:NO₂ ratio supplied to the SCR catalyst. Thus estimating the amount of ammonia required under transient conditions is challenging. Transient conditions are experienced under normal driving conditions and drive cycles, for example either the FTP75 drive cycle or

the new European drive cycle is used to assess the ability of a vehicle to comply with emissions legislation. There are many studies on transients in the literature, for example Wurzenberger et al. [1] where a rise and fall in ammonia level while NO remains constant is investigated. Olsson et al. [2] investigated step changes in NO and ammonia but at a fixed temperature on a reactor rig. Chatterjee et al. [3] looked at the simulation of complete test cycles. Indeed, ultimately it is necessary to be able to model the emissions from any particular exhaust system at any stage of the prescribed drive cycle. More recently Narayanaswamy et al. [4] looked at modelling transients obtained from experiments on a reactor rig for both iron and copper zeolite. Sharifian et al. [5] have studied iron zeolite transients but again under laboratory conditions.

As an approach to modelling transients, some engine tests have been performed that have provided measured emissions during simple transients. An attempt has then been made to try to predict these emissions using a CFD model. SCR kinetics available in the open literature have been used but the kinetics have been modified for the type of catalyst used [6]. These tests have been performed on a real engine with a real exhaust system but with 1D geometry to simplify the modelling. Simplified transients were investigated by ramping up at 1500 rpm from a low load, 6 bar bmep, holding for a period of time at a higher load, 9 or 10 bmep, and then ramping down again to the initial load. The ammonia supply rate was maintained at a fixed value during this procedure. This imitates what may happen in a vehicle under a sudden acceleration or deceleration when the engine load will change rapidly but the ammonia supply may not respond quickly enough to the change in conditions. Further studies have investigated rising engine load ramps and falling ramps separately. The studies here provide an investigation of very simple engine load ramps on a real engine system and explore how well an SCR kinetic scheme can describe the detail of the observations. Only if the detail in such experiments can be simulated correctly will modelling a full drive cycle produce accurate predictions throughout.

KINETICS AND MODELLING

The kinetics used for modelling SCR are essentially the scheme provided by Olsson et al. [2] for Cu-ZSM-5 zeolite. The SCR scheme consists of four reactions, commonly referred to as the standard reaction, the fast reaction, the slow reaction and N₂O formation. The equations for these are as follows:

- $4\text{NH}_3 + 4\text{NO} + \text{O}_2 \rightarrow 4\text{N}_2 + 6\text{H}_2\text{O}$
- $2\text{NH}_3 + \text{NO} + \text{NO}_2 \rightarrow 2\text{N}_2 + 3\text{H}_2\text{O}$
- $8\text{NH}_3 + 6\text{NO}_2 \rightarrow 7\text{N}_2 + 12\text{H}_2\text{O}$
- $2\text{NH}_3 + 2\text{NO}_2 \rightarrow \text{N}_2 + \text{N}_2\text{O} + 3\text{H}_2\text{O}$

NO and ammonia oxidation reactions are also both included in the scheme, although these have modest influence at the

relatively low temperatures investigated here, in the range 200 to 300°C. Ammonia adsorption and desorption are particularly important in transient simulations. Olsson's form of the ammonia desorption reaction has an activation energy that is dependent upon the ammonia coverage of the active sites. Olsson et al. use 200 mol sites/m³ as the value for the number of sites in their catalyst. The maximum available sites that can be occupied by stored ammonia is a function of temperature, but the balance between adsorption and desorption in the Olsson expressions caps the maximum value of θ at any particular temperature, i.e. it fixes the fraction of sites occupied, and hence accounts for the change in storage capacity with temperature. It is possible to model this differently by using a temperature dependent value for the number of sites $\Omega(493/T)^2$, in which case the sites can reach full occupancy. This is an alternative to the assumption of a fixed site density that is independent of temperature. This means that fraction θ is not precluded from attaining the value unity at all temperatures. In order to simulate the transients here, this methodology has been followed and ammonia desorption has been reformulated so that it is negligible at the temperature of the experiments. Ammonia can still be removed from the sites by reaction.

The model is based on the porous medium approach, [7], where the catalyst brick is represented by an analogous porous medium. The modelling here is in 1D as the engine experiments are 1D, see below, but with the porous medium approach a developed model can readily be applied to three dimensional cases. The model was run in Star-CD software. The scalar species modelled were oxygen, NO, NO₂, NH₃ and N₂O. These had distinct concentrations both in the gaseous and pore phases in the CFD model. Mass transfer between the bulk stream and the wall was accounted for by source terms based on transfer coefficients and coded into a user subroutine. Source terms based on reaction rates allowed consumption of species in the pore phase. The ammonia storage θ was also dealt with as a pore phase species. This is interpreted within the Star-CD CFD model by Eq. (1), where the net rate of storage of ammonia is then found from the balance between adsorption, desorption and consumption. This equation is solved along with those for the other species.

$$\varepsilon p_{\text{Air}} \frac{\partial \theta}{\partial t} = \frac{\varepsilon p_{\text{Air}}}{\Omega} [R_{\text{ads}} - R_{\text{des}} - R_{\text{con}}] \quad (1)$$

In the equation the reaction rates are in mol/m³ monolith/s and the ammonia capacity of the substrate has value Ω mol-sites/m³ monolith. Enthalpy source terms were not accounted for in the simulations as the net effect of the SCR processes is minimally exothermic and the consequent temperature changes are only one or two degrees at most.

The computational mesh used for the 1D CFD simulations consisted of a rectangular block of cells, with the cells in the

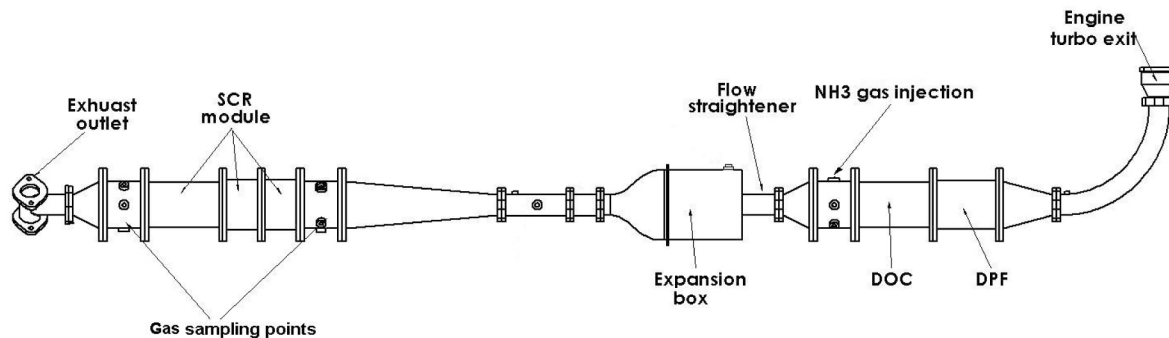


Figure 1. Exhaust system on engine test rig.

porous medium having length near 2mm. The PISO algorithm was used for the transient simulations and the time steps were of order 0.01 s during the transient. Each simulation of the transient experiment was preceded by a run for 900 s of real time to simulate the engine being run to steady state in the tests.

METHODOLOGY OF TRANSIENT ENGINE TESTS

The engine test rig exhaust system is shown in [Figure 1](#). The 2.0 litre Diesel engine was run without EGR so that NO_x levels were high and readily measureable. The DPF was placed upstream of a DOC; this is a non-standard configuration. The length of the DOC was used to control the NO₂:NO_x ratio and the possibility of reaction between NO₂ and soot on a downstream DOC was avoided. Ammonia gas was injected upstream of a flow straightener, expansion box and converging nozzle. This ensured good mixing of the ammonia with the exhaust stream and the supply of a uniform velocity profile to the inlet of a long ten-degree diffuser cone. This in turn supplied a uniform velocity profile to the inlet of the SCR catalyst brick, so that the experiments were in effect one-dimensional. Different lengths of brick could be fitted into the exhaust as the fittings were modular. The SCR catalyst used in these experiments was a form of copper zeolite. The test exhaust was fitted with instrumentation sampling ports as indicated in [Figure 1](#). The gas analysis instrumentation was either a fast response, 2.0 ms, Cambustion CLD analyser that could measure NO and NO₂ or a Horiba 6000FT gas analyser that could measure additionally N₂O. The Horiba analyser had a slower response and in experiments where that analyser was used the data was logged at 1 second intervals. The data was logged at 0.01 s intervals during the transient when the fast CLD analyser was used.

Although the engine test rig exhaust was specially designed and different from a regular exhaust system, nevertheless the transients studied were typical of real systems. The porous medium model developed, which is based on the experiments

on this rig, will be applicable to real systems as discussed in the previous section.

Tests Where Engine Load was Ramped Up and Down

Two types of tests were carried out. In the first set that used the fast response analysers, the engine was allowed to reach steady state. [Table 1](#) summarises the initial steady state conditions for this set of tests. After 20 seconds logged at steady state in every case, the engine was ramped up from 1500 rpm, 6 bar to 1500 rpm, 9 bar over the prescribed time period of either 10 s or 20 s. The engine was then held at the higher load condition for the same prescribed time period and was then ramped down, also over the same prescribed time period. For these tests the SCR brick was made up of two short bricks, 45 mm plus 45 mm in length, so that in effect a full 91 mm length SCR was used. The DOC was either 45 mm long, referred to as 0.5 DOC, or 91 mm long, referred to as 1.0 DOC. This gave two different NO₂:NO_x conditions; the NO₂:NO_x ratios varied during the experiments and their traces are shown for reference in [Figure 2](#). As the engine load rises, the NO level increases but the NO₂ increase is dependent upon the temperature rise and the response of the DOC to the change in conditions. This accounts for the shape of the NO₂:NO_x ratio curves in [Figure 2](#).

The Cambustion NO_x analyser is sensitive to cross talk by ammonia so measurements were made only downstream of the SCR using this analyser in this set of tests. Furthermore, the dosing of ammonia was deficient so that ammonia levels downstream of the SCR observed in the experiments were never more than a few ppm. The temperatures upstream of the SCR during these tests are shown in [Figure 3](#). [Figure 3](#) shows that the temperature change that occurs is quite small when a rising ramp is followed quickly by a falling ramp as the higher load is not maintained for long enough for a high temperature to become established. It should be noted that the mass flow rate of exhaust varied during the transients because the engine operating condition changed. The ammonia level in the exhaust upstream of the SCR was measured initially under steady state conditions at the lower engine load and

nominally was held steady at this level throughout the experiment. However, as the mass flow rate increased, the ammonia level decreased during the transient phase of each experiment because of dilution. This change in ammonia level was accounted for throughout the simulation because the instantaneous mass flow rate was available as input.

Table 1. Summary of initial conditions for the ramp up and ramp down transient tests for 10 s and 20 s cases.

	0.5 DOC (20 s)	1.0 DOC (20 s)
T deg C	214.8	213.0
MF kg/hour	109.0	110.0
% O ₂	11.1	11.3
NO ppm	430	266
NO ₂ ppm	164	275
NH ₃ ppm	282	282
Initial NO ₂ :NO _x %	27.6	50.8

	0.5 DOC (10 s)	1.0 DOC (10 s)
T deg C	214.0	213.0
MF kg/hour	109.0	110.5
% O ₂	11.1	11.4
NO ppm	427	267
NO ₂ ppm	155	275
NH ₃ ppm	282	283
Initial NO ₂ :NO _x %	26.6	50.7

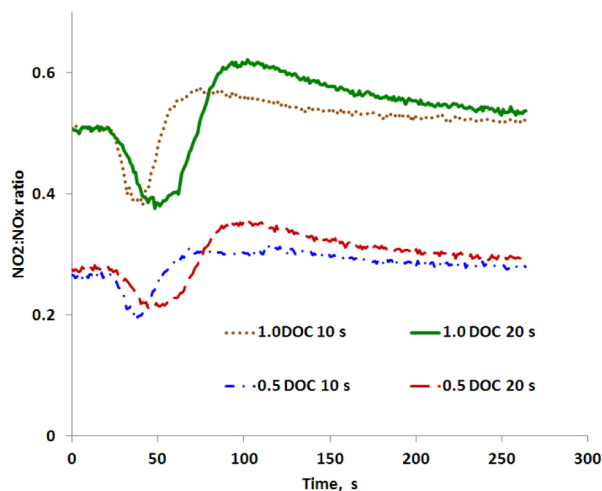


Figure 2. NO₂:NO_x ratios during the ramp up and ramp down tests.

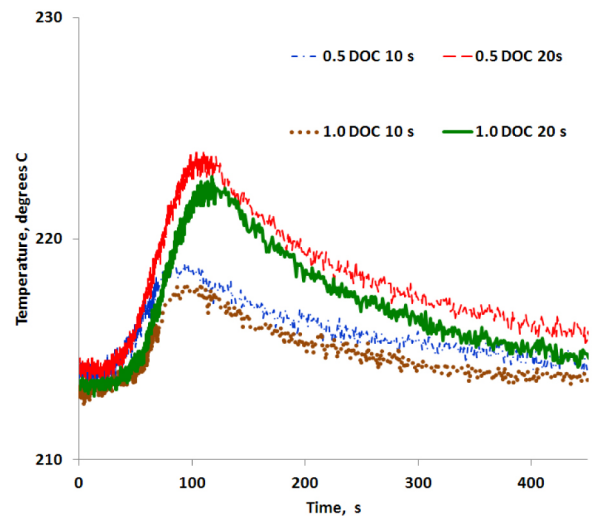


Figure 3. Temperatures at SCR inlet during the ramp up and ramp down tests.

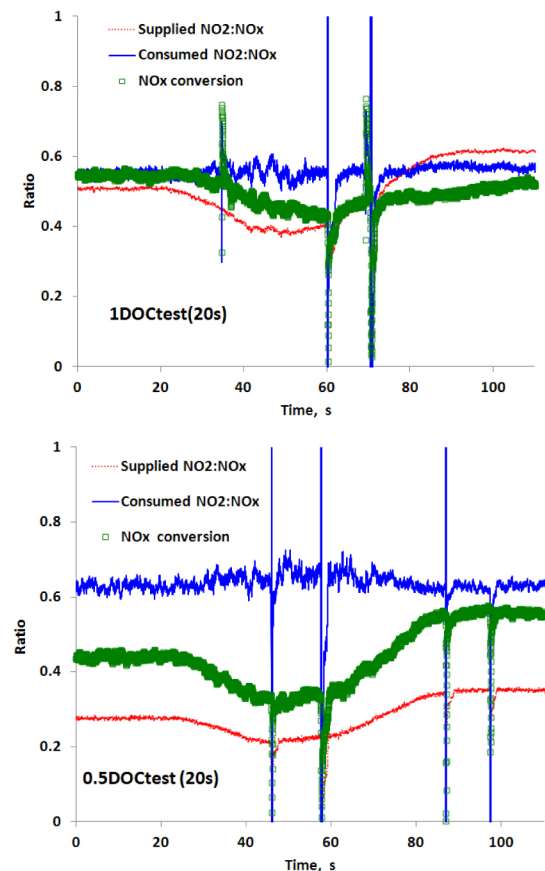


Figure 4. Data plots showing that consumed NO₂:NO_x ratio is independent of supplied NO₂:NO_x ratio during the transient. Spikes are instrumentation blips from the CLD analyser and are not significant.

Figure 4 shows the measured consumed ratios during the 20 s transient between 0 and 100 s when the supplied NO₂:NO_x ratio is changing. For the 1 DOC case the supplied ratio is about 0.5 and the consumed ratio is slightly higher but

remains constant during the transient part of the test. For the 0.5 DOC case, the supplied ratio is initially near 0.25 but the consumed ratio is above 0.6 and again remains approximately constant during the transient part of the test. When the NO₂:NO_x ratio supplied is near 0.5, NO_x conversion is near 50 % throughout whereas when proportionately less NO₂ is present, conversion is just over 40 % at the start, drops to near 30 % but then rises to near 60 % by the end, at which point the supplied NO₂:NO_x has also risen, although it is still well below 50%.

Tests Where Engine Load was Ramped Either Up or Down

In the second set of tests, the engine was ramped up from 1500 rpm, 6 bar to 1500 rpm, 10 bar over 20 seconds and the higher load was then maintained until steady state was achieved. The engine load was then ramped down again over 20 seconds and the lower load was maintained until steady state conditions were achieved. These tests used the FTIR analyser, so there was no restriction on the level of ammonia that could be used in these experiments. The SCR brick length was only 45 mm in this case and the DOC was a Pd DOC so that only NO was supplied to the SCR during these tests [8]. The temperature achieved in these tests was much higher because the engine load was maintained at the higher level for a longer period of time, see Figure 5.

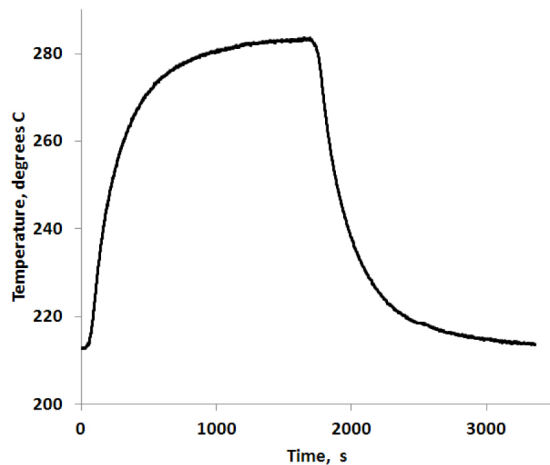


Figure 5. Temperature at SCR inlet during rising ramp and falling ramp tests.

RESULTS

Tests Where Engine Load was Ramped Up and Down

In these tests, both NO and NO₂ were supplied to the SCR and the measurements were made using the fast response CLD analysers. Figure 6 shows the experimental data and simulations for the 0.5 DOC, 10 s transient experiment. These

simulations used the Olsson et al. scheme [2]. The NO level downstream is under-predicted, i.e. there is more NO conversion in the simulation than in the experiment. The NO₂ level is over-predicted, which means that the simulation has underestimated the conversion of NO₂.

Figure 7 shows a significant improvement in agreement. This has been achieved by a modification to the kinetic parameters of the standard SCR reaction and adjustments to ammonia adsorption and desorption rates as documented in [6] and as discussed later in this paper. It has, however, been necessary also to increase the rate of the so-called slow reaction by a factor of 20. This has improved agreement of both NO and NO₂ although there is still a small discrepancy at the peak of the transient.

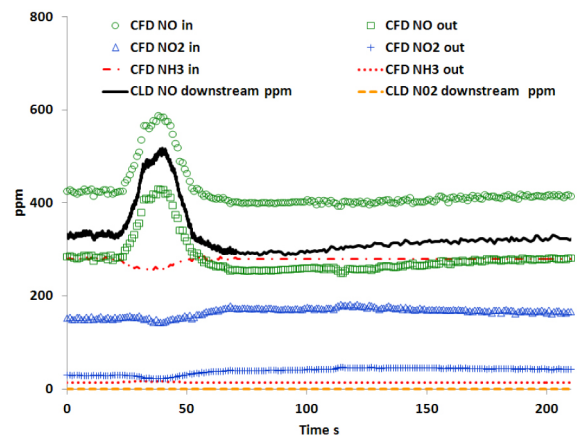


Figure 6. 0.5 DOC, 10 s transient simulation using unmodified Olsson kinetics [2] with Ω fixed at 200 mol sites /m³.

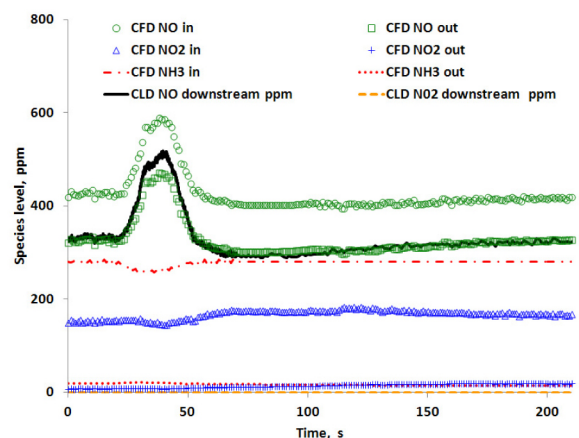


Figure 7. 0.5 DOC, 10 s transient simulation using modified kinetics and multiplier 20 applied to the slow reaction.

Figure 8 shows the experimental data and simulations for the 1.0 DOC, 10 s transient experiment. These simulations used the Olsson et al. scheme [2]. The NO level downstream is

moderately well predicted but the NO_2 level is over-predicted, which means that the simulation has underestimated the conversion of NO_2 .

Figure 9 shows only a slight improvement in agreement when compared with Figure 8. This was achieved by a modification to the kinetic parameters of the standard SCR reaction and changes to ammonia adsorption and desorption as documented in [6]. It has, however, not been necessary to increase the rate of the so-called slow reaction in this case. The Olsson kinetics seem to provide an adequate description of this case where the supplied $\text{NO}_2:\text{NO}_x$ ratio was near 50 % and the kinetics were dominated by the fast reaction. The modified standard rate kinetics contributed a small improvement but the standard, slow and N_2O reaction rates were less important in this case.

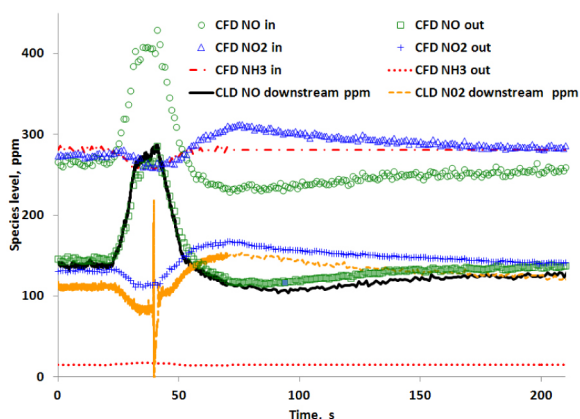


Figure 8. 1.0 DOC, 10 s transient simulation using unmodified Olsson kinetics [2] with Ω fixed at 200 mol sites/m³.

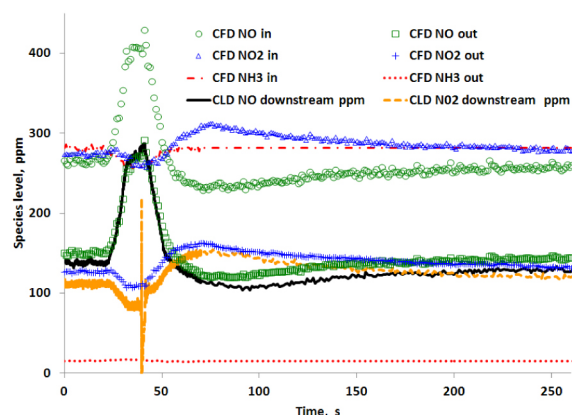


Figure 9. 1.0 DOC, 10 s transient simulation using modified kinetics and multiplier x1 applied to the slow reaction.

Figure 10 is for the 0.5 DOC and 20 s transient simulated using modified kinetics and can be compared with Figure 7 for the 10 s transient. The longer transient in Figure 10 shows a similar disagreement at the peak as noted in Figure 7, but there is also a small disagreement of NO levels later in the simulation. The predicted output NO_2 level is notably higher after 100 seconds than the measured level. Increasing the slow reaction rate further in the simulation did remedy this, but the agreement between measured and simulated NO level then deteriorated.

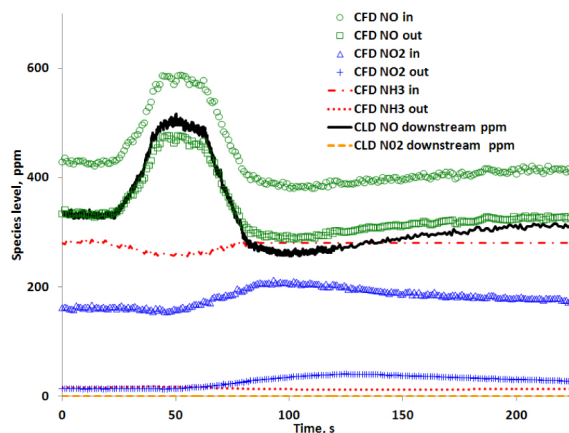


Figure 10. 0.5 DOC, 20 s transient simulation using modified kinetics and slow rate SCR multiplier x 20.

Figure 11 is for the 1.0 DOC and 20 s transient simulated using modified kinetics and can be compared with Figure 9 for the 10 s transient. The longer transient in Figure 11 shows a similar degree of agreement between measurements and predictions, with both NO and NO_2 agreeing fairly well. The fast reaction dominates in this case and so either the Olsson scheme or the revised scheme can give a reasonable prediction.

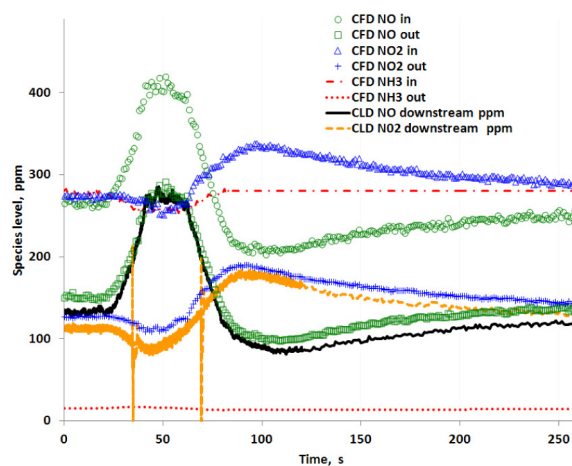


Figure 11. 1.0 DOC, 20 s transient simulation using modified kinetics and slow rate SCR multiplier x1.

Tests Where Load was Ramped Either Up or Down

The measurements for these tests were obtained using the FTIR analyser. The results for the upward ramp in the second set of tests are shown in Figures 12 and 13. Only NO was supplied to the SCR in these tests as the Pd DOC was used in the exhaust. Figure 13 shows the case using revised kinetics and Figure 12 shows the case using Olsson kinetics. The improvement in this case between Figures 13 and 12 can be seen very readily. In Figure 12 the conversion of both ammonia and NO is severely over-predicted whereas in Figure 13 the agreement is very good.

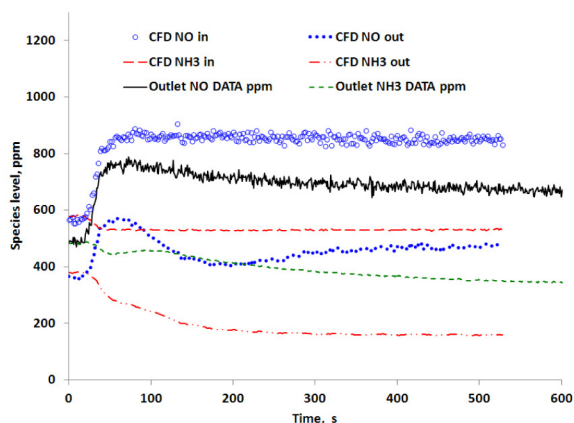


Figure 12. Upward ramp in Pd DOC test simulated using Olsson kinetics [2] with Ω fixed at 200 mol sites /m³.

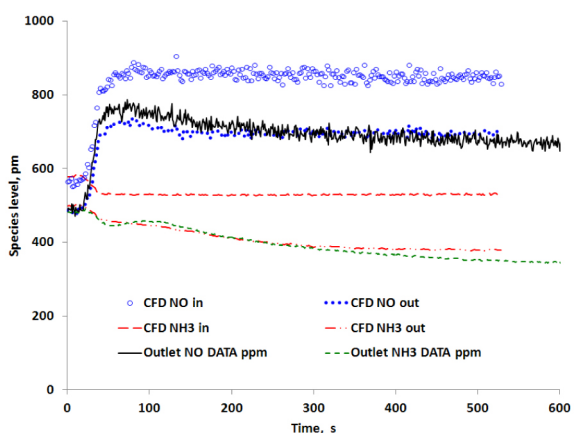


Figure 13. Upward ramp in Pd DOC test simulated using modified kinetics.

The results for the downward ramp in the second set of tests are shown in Figures 14 and 15. Figure 15 shows the case using revised kinetics and Figure 14 shows the case using Olsson kinetics. The improvement in this case between Figures 14 and 15 can again be seen very readily. In Figure 14 the conversion of both ammonia and NO is severely over-predicted for the downward ramp as it was for the upward

ramp. In Figure 15 the agreement is very good, particularly for NO.

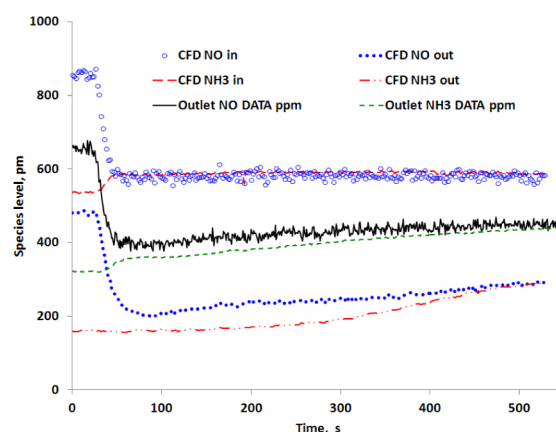


Figure 14. Downward ramp in Pd DOC test simulated using Olsson kinetics [2] with Ω fixed at 200 mol sites /m³.

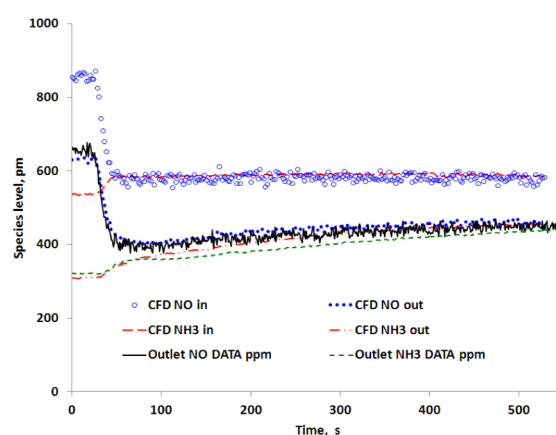


Figure 15. Downward ramp in Pd DOC test simulated using modified kinetics.

DISCUSSION AND CONCLUSIONS

The kinetic modifications to the standard reaction rate were based on some studies using the Pd DOC [6] so that the NO_x in the engine exhaust was mainly NO. These modifications are summarised in Table 2.

The modifications included changing the adsorption multiplier. This had to be adjusted to provide the best agreement in different cases and a universally applicable value has not yet been established for the catalyst being used. Tuning the adsorption with the multiplier and with the exponential term in place of (1- θ) had strong influence on the rising ramp or falling ramp tests carried out with the Pd DOC, but was apparently less important in the rising and falling ramp tests, where the temperature change was smaller. This multiplier may be a function of temperature but further tests would be required to establish this.

Table 2. Olsson and modified kinetics

	Olsson kinetics	Modified kinetics
k; E for std. reaction	2.3E+08; 84.9 kJ/mol	8.93E+05; 63.484 kJ/mol
Local ratio applied to std. reaction	-	NO/(NO+NO ₂ +NH ₃)
Adsb. multiplier	0.93	0.93 (Pd DOC; upward ramp) 1.86 (Pd DOC; downward ramp) 3.2 (0.5 DOC and 1.0 DOC; upward & downward ramp tests)
Adsb. θ term	(1- θ)	exp(-3 θ)
Coverage dependence of desorption activation energy	(1-0.98 θ)	(1-0.2 θ); desorption negligible at experiment temperature
Capacity, Ω	200 mol sites/m ³	90(493/T) ² mol sites/m ³ in the range 473 – 573 K

The experiments reported in this paper were fairly low temperature engine load ramp tests with exhaust temperatures between 200 and 300 degrees C, typical of passenger car Diesel exhausts. In these tests the ammonia dosing was kept approximately constant, although there was a small change in concentration due to mass flow rate change during the transient. In the experiments with 0.5 or 1.0 DOC it was noted that the consumed ratio of NO₂:NO_x remained approximately constant during the transient even though the supplied NO₂:NO_x ratio was changing.

The tests carried out with a Pd DOC were separate upward and downward ramps, and the exhaust NO_x was composed of NO only. It proved possible to obtain very good predictions of species levels downstream of the SCR by modifying the standard reaction rate and the ammonia adsorption rate in the kinetic scheme. Ammonia desorption was negligible at the temperature of the simulations, i.e. in effect it was turned off. This was reasonable at these temperatures and under these conditions. In the simulation ammonia was removed from storage by reaction but not by spontaneous desorption.

The tests carried out with 0.5 DOC and 1 DOC supplied some NO₂ as well as NO to the SCR. When this mix was 50 % NO and 50 % NO₂ then either the Olsson kinetics or the modified kinetics seemed to be comparable in their ability to predict the downstream species levels. Both gave reasonable predictions. This was because the fast reaction dominates under these conditions and this rate is not changed in the modified kinetic scheme. The influence of the other three SCR reactions was minimal. When 25% of the NO_x was NO₂ then the kinetic scheme required modification. The modified standard reaction kinetics together with changes to the adsorption were implemented. However, the slow reaction rate also had to be promoted by a factor of 20 in the simulations in order to increase the consumption of NO₂ and thereby achieve the balance between NO and NO₂ consumption that was observed in the experiments. A factor of 20 is at the upper limit of what might be considered to be a reasonable change. It may be that the slow reaction should be adjusted by a more reasonable factor of 4 or 5 and that the

N₂O formation reaction should also be increased by a factor in order that sufficient NO₂ is consumed in the model. The latter could be confirmed by N₂O measurement and this is planned for future studies. The main point is that NO₂ is observed to be consumed in larger amounts than expected and a change is required to the kinetic scheme to account for this.

This research is ongoing and further tests of the type described in this paper are currently in progress. Tests of the second type with separate upward ramp and downward ramp but using 0.5 and 1.0 DOC, so that the supply is a mixture of both NO and NO₂, are underway. The results of these tests may help to further clarify the changes needed to the kinetics in order to obtain a universal description of the observations. At present it is necessary to make adjustments to the ammonia adsorption parameter in order to obtain very good agreement. Also, the amount by which the slow reaction rate needs to be enhanced in order to obtain good predictions when NO₂ is present in quantities less than 50 % requires further investigation.

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DEFINITIONS/ABBREVIATIONS

Rads - Rate of NH₃ adsorption

Rdes - Rate of NH₃ desorption

Rcon - Rate of NH₃ reaction

ε - Porosity fraction

θ - Site coverage fraction

ρ - Density(kg/m³)

Ω - Capacity(mol sites/m³)

t - Time (s)

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