

Experimental and kinetic modelling of DPF and SCR coated filters

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Highlights

- Addition of soot did not influence the catalytic activity of Cu/SSZ-13 during standard SCR conditions.
- Water increased, while ammonia negatively influenced the soot oxidation
- Kinetic model for DPF and soot coated Cu/SSZ-13 was developed

1. Introduction

Ammonia Selective Catalytic Reduction (NH₃ SCR), is one of the most efficient post combustion abatement technologies for removing NO_x from diesel engines [1,2]. To remove soot, diesel particulate filters (DPF) are used. Recently, SCR coated filters have been introduced, which capture soot and simultaneously are active for ammonia SCR [3]. There are large advantages with using SCR coated filters, such as decreased volume and better light off characteristics.

2. Methods

The impact of soot on Cu/SSZ-13 in standard SCR, NH₃ oxidation, NH₃ temperature programmed desorption (TPD), as well as soot oxidation in a presence of water were examined using flow reactor measurements. Experiments were done in two steps over the Cu/SSZ-13 monoliths, where the activity on fresh Cu/SSZ-13 was first examined. Thereafter, a mixture of soot powder (generated at engine bench at Volvo Cars) and ethanol was impregnated on the Cu/SSZ-13 samples. Then ethanol was removed and activity was measured again. Moreover, soot oxidation experiments on soot loaded Cu/SSZ-13 were done in a presence of 8% of O₂ and in a presence of 8% of O₂ and 5% H₂O.

Kinetic models were developed using AVL Boost. The impact of different gases, such as ammonia and NO on the soot oxidation was simulated using experimental data for temperature ramp experiments over small DPF samples, that contained soot from engine bench experiments at VCC [4].

3. Results and discussion

The soot oxidation over Cu/SSZ-13 in different gas atmospheres was studied and the amount of CO and CO₂ produced in each experiment is used to calculate the soot oxidized at each temperature as presented in Figure 1.

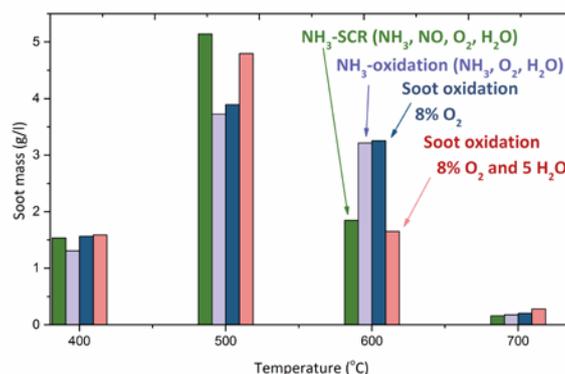


Figure 1. Integrated CO and CO₂ result for soot oxidation over Cu/SSZ-13 samples.

The influence of water on soot oxidation shifts the maximum of CO₂ and CO production towards lower temperatures, thus water increases the soot oxidation. When adding ammonia to the system it is clear that the soot oxidation is lowered in the presence of ammonia, resulting in larger integrated CO_x at 500°C for O₂+H₂O, while opposite results at 600°C were received where more was oxidised for O₂+H₂O+NH₃. Interestingly, during ammonia SCR conditions the activity for soot oxidation is regained at 500°C. At this high temperature, the SCR zone is very short, thus the majority of the catalyst is not exposed to ammonia and therefore the inhibition effect of ammonia is not observed.

A kinetic model for the effect of gas composition for soot oxidation was developed using experimental data on DPF and an example of results are shown in Figure 2, where soot is oxidised in the presence of NH₃, NO, O₂ and H₂O. The developed model was thereafter used to model SCR coated filters and the model could well describe the experimental findings.

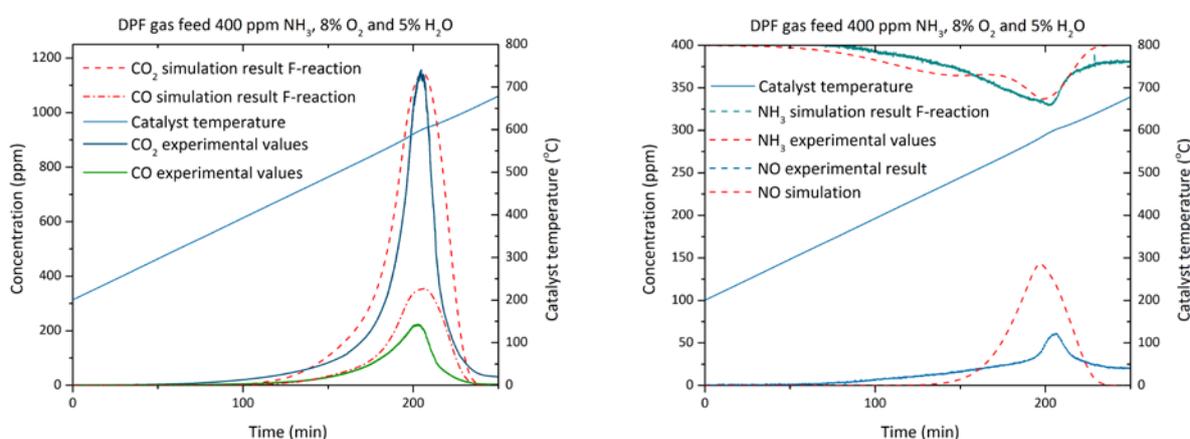


Figure 2. Kinetic model for NH₃ effect on soot oxidation over DPF.

4. Conclusions

The addition of soot did not influence the catalytic activity of Cu/SSZ-13 during standard SCR. Water increased the soot oxidation while ammonia negatively influenced it. Ammonia SCR conditions increased the soot oxidation compared to ammonia oxidation, because NH₃ is quickly being removed in the SCR reaction. Kinetic models for DPF and soot coated Cu/SSZ-13 was developed and could well describe the experimental features. Important features in the model are: (i) pore growth model for describing the growth of soot pores with random size distribution (ii) Ammonia inhibition on important free edge sites (supported by DRIFT data for amid—species) and (iii) NO formation over soot.

References

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Keywords

Soot, Kinetic modeling, DPF, SCR coated filters.