REWARD

REal World Advanced Technologies foR Diesel Engines

EUROPEAN COMMISSION
Horizon 2020
H2020-MG-2014-2015
GA No. 636380

Deliverable No.	REWARD D2.3	
Deliverable Title	SCRF model, including regeneration	
Deliverable Type	REPORT	
Dissemination level	Confidential – member only (CO)	
Written By	LIDIJA TRANDAFILOVIC AND LOUISE OLSSON (CTH)	2017-04-24
Status	**Final**	2017-05-15
Checked by	MARCO TONETTI (CRF) WP2 Leader	2017-05-01
Submitted to Executive Board	Submitted to all members of Executive Board	2017-05-02
Approved by Executive Board (EB)	Approved and accepted by all members of Executive Board	2017-05-12

H2020-MG-2014-2015 – 636380 – REal World Advanced Technologies foR Diesel Engines

Acknowledgement:

The author(s) would like to thank the partners in the project for their valuable comments on previous drafts and for performing the review.

Project partners:

1 - AVL - AVL List GmbH - AT
2 - REN - Renault SAS - FR
3 - VCC - Volvo Car Corporation - SE
4 - CRF - CRF SCpA - IT
5 - CNRIM - Instituto Motori – Consiglio Nazionale delle Ricerche (CNR) - IT
6 - JM - Johnson Matthey Plc - UK
7 - RIC - Ricardo Plc - UK
8 - SCF - Schaeffler AG - DE
9 - LMM - Le Moteur Moderne - FR
10 - DELPHI - Delphi Automotive Systems Luxembourg S.A. - LU
11 - UNR - Uniresearch BV - NL
12 - IFPEN - IFP Energies Nouvelles - FR
13 - VIF - Virtual Vehicle Research Center - AT
14 - CTH - Chalmers Tekniska Högskola - SE
15 - CTU - Czech Technical University - CZ
16 - UPVLC - Universitat Politecnica de Valencia – Motores Termicos - ES

Disclaimer:

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 636380.

Publishable Executive summary

SCR coated particulate filter is a device that captures soot and simultaneously is active for ammonia SCR. There are large advantages with using SCR coated filters, such as decreased volume and also better light off characteristics, since both the SCR function as well as filter function is close to the engine. The objective of this work is to study the effect of soot on SCR coated filters and develop a kinetic model for this system.

Cu/SSZ-13 materials were synthesized and coated on monoliths. As synthesized, Cu/SSZ-13 samples were characterized with Brunauer-Emmett-Teller (BET) surface area analysis, X-Ray Diffraction (XRD) and elemental analysis conducted using an inductively coupled plasma sector field mass spectrometry (ICP-SFMS). The BET Surface Area of the Cu/SSZ-13 sample is 555.3 m^2/g. The result of ICP measurement show that Cu/SSZ-13 contain Si (34.7%), Al (6.08 %) and Cu (4.5 %). XRD confirmed the structure of the zeolite. The in situ diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) experiments were done to study ammonia storage on soot. A flow reactor was used to measure the activity for standard SCR, NH_3 oxidation, NH_3 temperature programmed desorption (TPD) and soot oxidation.

The flow reactor experiments showed that there was only minor effect of soot addition on the ammonia oxidation and ammonia SCR. Moreover, the ammonia storage and release was slightly influenced by the presence of soot. In order to better understand the influence of water and other elements (NH_3, NO) on soot oxidation, the amount of CO and CO_2 produced in each temperature step is calculated and on the basis of these measurements, the total soot loading for our experiments was roughly 10 g/L. These results show that water promotes the soot oxidation. Another interesting effect, is the addition of ammonia. When comparing the results for O_2+H_2O with O_2+H_2O+NH_3 it is clear that the soot oxidation is lowered in the presence of ammonia. To conclude the presence of ammonia reduces the soot oxidation. 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.

DRIFT result for soot sample without NH_3 and in the presence of NH_3 at 100 ^oC was performed. Interestingly, there is one band which do not overlap with gas ammonia and this is the NH_3 adsorption band 1100-1000 cm^{-1}, which is due to formation of amide –C-NH_2. To conclude, the band at 1100-1000 cm^{-1}, clearly show that there is an interaction between soot and NH_3.

A kinetic model for ammonia storage and release, ammonia oxidation and ammonia SCR was tuned to the experimental results using the following reaction steps:

Reaction	
Ammonia storage on S1	$S1 + NH_3 \Leftrightarrow S1 - NH_3$
Ammonia storage on S2	$S2 + NH_3 \Leftrightarrow S2 - NH_3$
Ammonia storage on S3	$S3 + NH_3 \Leftrightarrow S3 - NH_3$
Ammonia oxidation on S1	$2S1 - NH_3 + 1.5\, O_2 \Rightarrow N_2 + 3H_2O + 2S1$
Ammonia oxidation on S2	$2S2 - NH_3 + 1.5O_2 \Rightarrow N_2 + 3H_2O + 2S2$
Ammonia SCR on S1	$4S1 - NH_3 + 4NO + O_2 \Rightarrow 4N_2 + 6H_2O + 4S1$
Ammonia SCR on S2	$4S2 - NH_3 + 4NO + O_2 \Rightarrow 4N_2 + 6H_2O + 4S2$

S1 are sites in the six-membered ring of the zeolite, S1 are sites in the eight-membered ring of the zeolite, S3 are physisorption sites.

Moreover, a kinetic model for soot oxidation was developed using soot on a DPF. This model included the interactions between soot and ammonia and the model could describe the experimental features very well. In addition, this model was used to simulate the soot regeneration during ammonia oxidation and ammonia SCR over soot loaded Cu/SSZ-13. The model was also able to describe these experiments very well.