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Full Length Article

Application of a global kinetic model on an SCR coated on Filter (SCR-F) catalyst for automotive applications

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ABSTRACT

Selective Catalytic Reduction (SCR) catalysts coated on diesel particulate Filter, SCR-F, have been introduced for automotive applications in the last years due to the capability of reducing NO_x and PM simultaneously below the limits imposed by emission regulations. In this context, the performance of a commercial silicon carbide Cu/zeolite SCR-F for controlling NO_x emissions in an automotive diesel engine was analyzed both experimentally and numerically for different soot loading levels with the aim to investigate its catalytic properties and to build a simulation model of the aftertreament device capable of predicting NO_x conversion efficiency, NH_3 storage capacity and soot conversion due to passive regeneration.

1. Introduction

One of the main issues associated with automotive diesel engines is undoubtedly represented by their high NO_x emissions, and the upcoming stringent emission regulations invoke the necessity of reliable aftertreatment systems capable of reducing NO_x to levels below the legislation limit [1–3].

Selective Catalytic Reduction (SCR) catalysts are one of the most promising technologies for controlling NO_x emissions with acceptable efficiency over a wide range of temperatures by using ammonia as an active intermediate for NO_x reduction. Ammonia is provided to the system through urea decomposition which is injected into the exhaust line upstream of the catalyst. NO_x reduction with ammonia is mainly controlled by the three SCR reactions expressed in Eq. (1), which are usually referred as standard, fast and slow SCR. The SCR reaction kinetic highly depends on temperature and NO_2/NO_x ratio [4,5].

$$\begin{cases} \textit{Standard SCR}: & 4NH_3 - Z + 4NO + O_2 \rightarrow 4N_2 + 6H_2O + 4Z \\ \textit{Fast SCR}: & 2NH_3 - Z + NO + NO_2 \rightarrow 2N_2 + 3H_2O + 2Z \\ \textit{Slow SCR}: & 4NH_3 - Z + 3NO_2 \rightarrow 3.5N_2 + 6H_2O + 4 \end{cases} \quad (1)$$

Recently, Selective Catalytic Reduction (SCR) catalysts [6] coated on Diesel Particulate Filters (DPF) [7], often referred to as SCR-Fs, have been introduced for automotive applications due to capability of reducing NO_x and PM simultaneously, as depicted in Fig. 1. Moreover, as a result of combining different aftertreatment components, in SCR-F technology reduced packaging volume and cost [8], in addition to lower thermal capacity [9] and faster warm-up [10] for automotive applications are obtained.

Several studies have been carried out on SCR-F applications and modeling. As an example, Schrade et al. [11] developed a global kinetic model based on Synthetic Gas Bench (SGB) experimental data. Colombo et al. [12], transferred an existing SCR kinetic model into the wall of a DPF to assess the impact of soot on DeNOx activity and also SCR coating effect on soot conversion efficiency. Another SCR-F model was developed by Watling et al. [8], through the combination of an SCR kinetic model of a flow-through monolith and a physical model of a coated DPF, assuming that SCR coating does not affect soot oxidation kinetics.

In this paper the performance of a commercial Silicon Carbide Cu/zeolite Selective Catalytic Reduction coated on Filter (SCR-F) device for controlling NO_x emissions for automotive diesel

Abbreviations: cpsi, cell per square inch; DPF, Diesel Particulate Filter; SCR, Selective Catalytic Reduction; SCR-F, Selective Catalytic Reduction coated on Filter; SGB, Synthetic Gas Bench; TPD, Temperature Programmed Desorption; TPR, Temperature Programmed Reduction; UEGO, Universal Exhaust Gas Oxygen.

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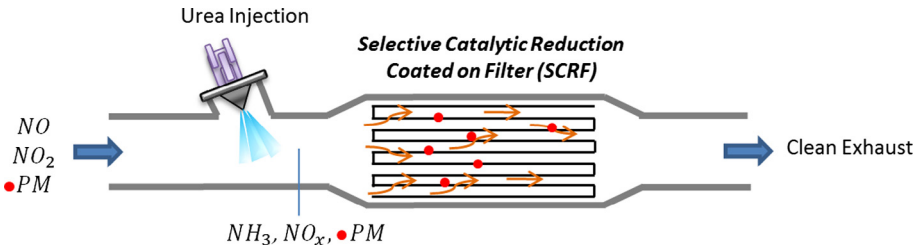

Fig. 1. SCR-F operating principle.

applications was analyzed, with the aim to investigate its catalytic properties and to build a simulation model of the aftertreatment device capable of predicting NO_x conversion efficiency, ammonia storage capacity and soot conversion due to passive regeneration.

2. Experimental Set-up and methodology

The experimental activity was performed at ACA – Center for Automotive Catalytic Systems of the RWTH Aachen University through a Synthetic Gas Bench (SGB), as shown in Fig. 2a. The sample was put into an isothermal cylindrical reactor which was placed in a furnace and the gases were mixed from compressed gas cylinders using mass flow controllers. The test rig can host samples with a diameter not exceeding 20 mm and a length in the range of 50–180 mm. As depicted in Fig. 2b two thermocouples, 0.5 mm diameter each, were mounted in the gas flow upstream, TUS, and downstream, TDS, of the sample. Moreover, the temperatures at the sample central channel inlet, T1, middle (3 radial positions, T2, T4, T5), and outlet, T3, were also measured. An example of inlet and outlet gas temperatures for some tests is presented in Fig. 3, confirming the assumption of isothermal conditions due to negligible temperature difference between inlet and outlet, even for the soot loaded sample in which passive soot regeneration occurs.

Gas concentration measurements were performed with a multicomponent FTIR with 1 Hz sampling frequency. Moreover, lambda evaluation was performed via a Universal Exhaust Gas Oxygen (UEGO) sensor and calculation from feed gas.

The lab-scale samples were obtained from a full-scale monolith (the main characteristics of which are reported in Table 1). The catalyst sample is a Si/C washcoated with Cu/zeolite with a cell density of 300 cells per square inch cell and wall thickness of 0.012 in. (equivalent to 0.3 mm).

Soot loading was performed with a small displacement Yanmar diesel generator engine under constant load conditions by using the soot filter canning shown in Fig. 4b for parallel loading of up to 8 samples. The conditioning was done in oven at 200 °C for a duration of 1 h. (see Fig. 4)

Two different soot loadings were tested in this work, 0 and 8 g/l respectively. Soot distribution was assumed uniform throughout the sample. After the samples have been soot loaded, the following tests, which will be described hereafter, were performed on the SGB:

1. Temperature Programmed Desorption (TPD) Test
2. Temperature Programmed Reduction (TPR) Test

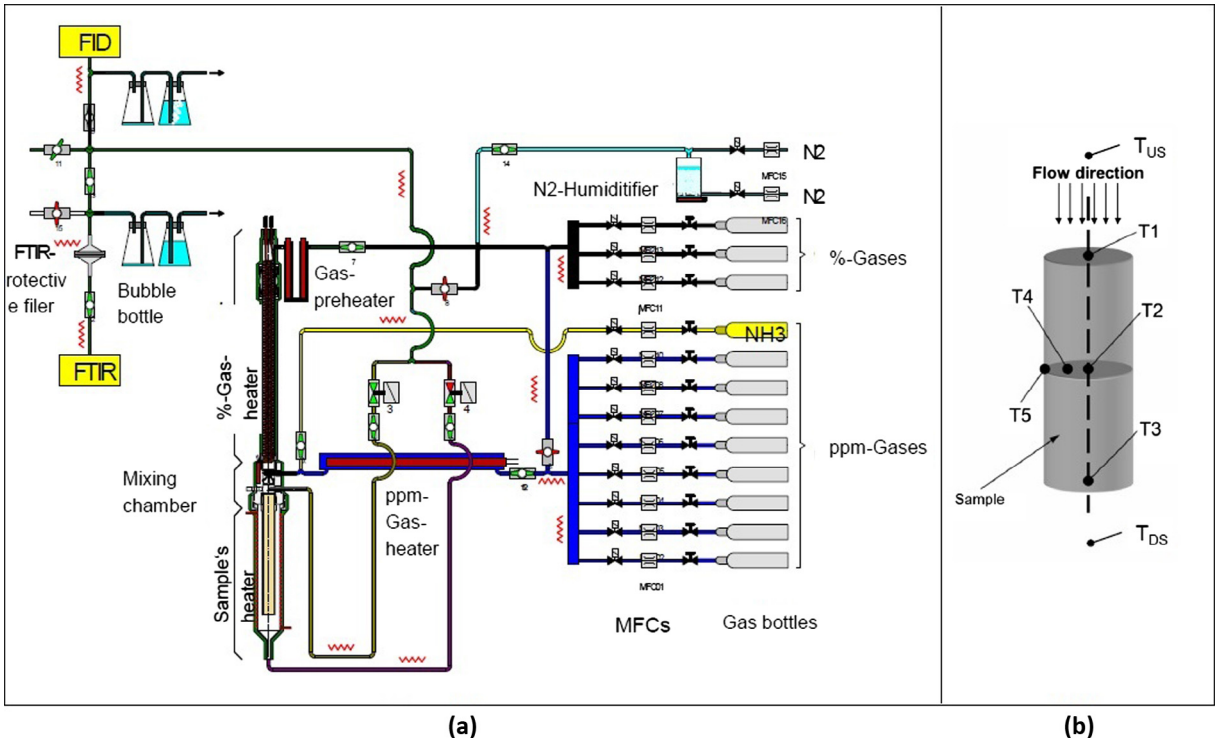

Fig. 2. Experimental setup: schematic view Synthetic Gas Bench (SGB) (a) and thermocouple locations on the lab scale sample (b).

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