Oxidation reactivity of (bio)diesel generated soot

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Soot oxidation reactivity is an essential parameter in automotive industry for optimizing engine parameters and designing exhaust aftertreatment systems. The more reactive a soot type is towards oxidation, the less energy is needed for the regeneration of a diesel particle filter. Under certain conditions it is even possible to continuously regenerate the particle filter at exhaust gas temperature (continuous regenerating trap CRT). Thus, for the development of an efficient exhaust aftertreatment system it is important to determine the optimal conditions and understand the underlying mechanisms of soot oxidation.

Additionally, there has been only little fundamental research on the impact of the use of biodiesel on soot oxidation reactivity. As the EU obligates the increment of the blending quota of biofuel to fossil fuel to up to 10 % until 2020 by the guideline 2009/28/EG, it is essential to study the impacts of parameters like blending quota of biodiesel to fossil diesel and engine parameters on soot structure and soot oxidation reactivity.

We study soot oxidation reactivity bv temperature-programmed oxidation (TPO, setup see Figure 1), which models the soot oxidation in a common diesel exhaust aftertreatment system. The soot-loaded filter sample is exposed to a gas flow at rising temperature from 373 to 973 K at a heating rate of 5 K min⁻¹. The gas flow simulates real exhaust composition and may contain besides O₂ and N₂ also other gases such as NO₂ and H₂O. The combustion emissions are monitored in dependence of applied temperature to the soot sample by FTIR spectrometry.



Figure 1. Scheme of TPO test bench.

By means of TPO, we studied the impact of different exhaust gas mixtures containing O_2 , H_2O and/or NO_2 on soot oxidation reactivity. Figure 2 shows the emission profiles of CO and CO_2 of commercial Printex XE2 soot (Degussa) in dependence of temperature and applied gas mixture. The temperature of maximum emission T_{max} can be used as criterion for soot oxidation reactivity (see Figure 2). It can be clearly demonstrated that NO_2 and H_2O are strongly increasing soot oxidation reactivity by shifting T_{max} towards lower temperatures.



Figure 2. TPO emission profiles of Printex XE2 soot analyzed under different oxidative conditions.

Raman microspectroscopy (RM) is furthermore applied to characterize the soot structure. RM is an established tool for the analysis of structural differences in the disordered (represented by Raman D band) and graphitic soot domains (represented by Raman G band) between different soot samples (Ivleva et al., 2007). Furthermore, the Raman spectra of soot exhibit a unique feature as the spectra of one sample differ in position and relative intensity of the D band when analyzed at different laser excitation wavelengths due to the dispersive character of the D band in soot spectra.

Final aim of this study is to analyze the soot oxidation reactivity by TPO under different conditions and correlate the TPO data with the structural information given by RM. Among others, a rapid and non-destructive method for the evaluation of the oxidation reactivity of biofuel generated soot by RM shall be established based on the method of multiwavelength Raman microspectroscopy (MWRM) for fossil fuel developed by Schmid *et al.* (2011).

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