Poster-Abstract

Development of a TGA-FTIR-method as R&D tool in exhaust gas aftertreatment

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The scope of this project is the development of a TGA-FTIR (Thermogravimetric Analysis and Fourier-Transformation-Infrared) method useful for research and development on exhaust gas aftertreatment systems.

This very strict emission limits for Diesel engines will lead to a combination of $DeNO_x$ systems and particulate filters in the future exhaust gas aftertreatment devices. However, the combination of these processes result in increasingly complex technical solutions and a superposition of various physical and chemical processes. Therefore, adequate analytical techniques are required in order to separate the different processes and to analyse single chemical reaction steps.

FTIR spectroscopy is a powerful analysis method for the gaseous reaction products out exhaust gas systems such as SCR catalysts or particulate filters. And TGA is very powerful for the investigation of adsorption and desorption processes on catalysts or soot samples. Therefore we intend to couple a FTIR spectrometer (Nicolet Antaris IGS by Thermofisher) and a TGA system (TGA/DSC 1 by Mettler-Toledo), which will be redesigned for research on exhaust gas aftertreatment systems. The instrument is equipped with a flexible gas supply system which gives us the opportunity to simulate real diesel exhaust gases in a broad range of compositions. The gas is supplied by 8 electronic mass flow controllers (MFC) operated by a LabView programm written in home. The standard gases dosed are N_2, NO, NO_2, NH_3, O_2 and H_2O plus SO2, CO and Hydrocarbons for special investigations. Water is generated by hydrogen oxidation over a Pt-catalyst at T > 250°C with N_2 as carrier gas, to which the other gas components are added. All tubes downstream of the water generation will be heated to prevent condensation. Condensation problems in the standard TGA instrument force us to redesign the inflow of the TGA.

Another challenge is the optimisation of the size and the shape of the gas cell of the FTIR spectrometer. A compromise has to be found between the need for small flow rates, which allows the detection of even small changes in the concentrations of the gas components, and a short residence time in order to prevent peak-broadening of the FTIR signals.

The system will be applied first to investigate the oxidation of soot and SCR on soot in parallel. And after that the urea decomposition will be examined with the apparatus in order to learn something about the to a large extent unknown mechanism.

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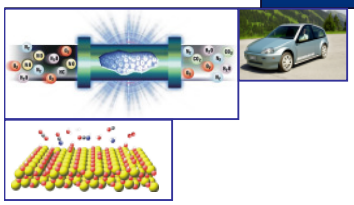

Development of a TGA-FTIR system as R&D tool in exhaust gas aftertreatment

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Motivation

The strict emission limits for Diesel engines will lead to a combination of DeNOx systems and particulate filters in the future exhaust gas aftertreatment devices. However, the combination of these processes result in increasingly complex technical solutions and a superposition of various physical and chemical processes. Therefore, adequate analytical techniques are required in order to separate the different processes and to analyse single chemical reaction steps.

The scope of this project is the development of a TGA-FTIR method useful for research and development on exhaust gas aftertreatment systems.

Elements of the apparatus

- TGA by Mettler Toledo
- FTIR spectrometer by Thermofisher
- 8 mass flow controller by Brooks, driven by a LabView program written in house
- Pt-catalyst for the generation of water by controlled hydrogen oxidation
- Computer for controlling TGA, FTIR spectrometer and the mass flow controller
- Heating system for the gas supply system and the transfer line to prevent condensation

System choice and resulting challenges

The combination of thermogravimetric analysis (TGA) and Fourier-Transform-Infrared (FTIR) spectroscopy is an efficient combination for R&D projects in the field of exhaust gas aftertreatment because TGA allows for investigation of adsorption and desorption processes and FTIR spectroscopy is suitable for analysis of gaseous reaction products with high resolution and long-term stability.

⟶ Resulting challenges and problems to be solved to use a TG-FTIR system as R&D tool for exhaust aftertreatment systems:

- Design of the gas supply
- Prevention of condensation of gas components ⟶ Redesign of the inflow of the TGA compared to the standard instrument
- Optimisation of size and shape of the gas cell of the FTIR spectrometer

First systems to analyse

The system will be applied first to investigate the oxidation of soot and the SCR reaction on soot in parallel:

soot oxidation: $2\,NO_2 + C \longrightarrow 2\,NO + CO_2$

standard-SCR: $4\,NH_3 + 4\,NO + O_2 \xrightarrow{cat} 4\,N_2 + 6\,H_2O$

NO_2-SCR: $4\,NH_3 + 3\,NO_2 \xrightarrow{cat} 3.5\,N_2 + 6\,H_2O$

„fast" SCR: $4\,NH_3 + 2\,NO + 2\,NO_2 \xrightarrow{cat} 4\,N_2 + 6\,H_2O$

Main questions:
- Which of the above mentioned SCR reactions occur on soot?
- What is the role of NH_4NO_3 deposited on the soot surface?
- Which side reactions have to be considered?

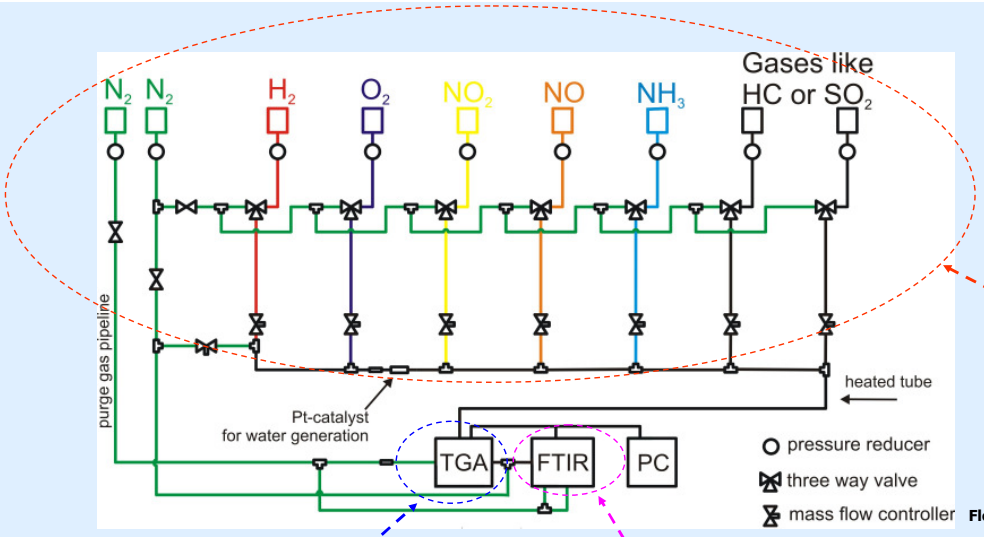
The decomposition of urea is another field of interest:

$(NH_2)_2CO + H_2O \xrightarrow{\Delta T} CO_2 + 2\,NH_3$

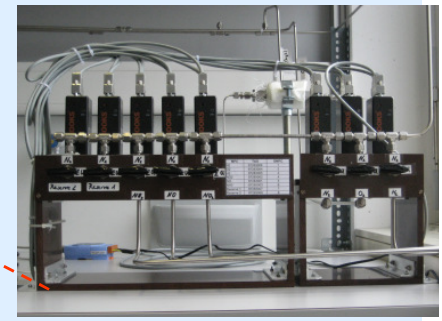
Main questions:
- What are the byproducts of urea decomposition?
- What is the underlying mechanism?
- Which role do catalysts play in the thermolyses of urea?

Specifications

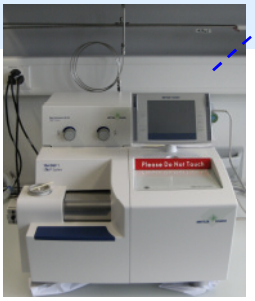
- Possibility to analyse the reaction products out of the exhaust gas aftertreatment systems down to very low concentrations
- Possibility to investigate adsorption and desorption processes on SCR catalysts or particulate filter materials
- Flexible gas supply for the simulation of real diesel exhaust gases in a broad range of compositions
- Fast switching between different compositions of the exhaust gases to simulate the dynamics of the diesel engine
- Trace-heated pipes to prevent condensation of exhaust gas components like H_2O and NO_2



Flow chart of the analytical system

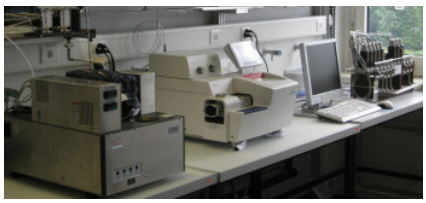


8 mass flow controller for the simulation of diesel exhaust gases



TGA/DSC 1, Mettler-Toledo

FTIR spectrometer, Thermofisher



Overview of the TGA-FTIR system