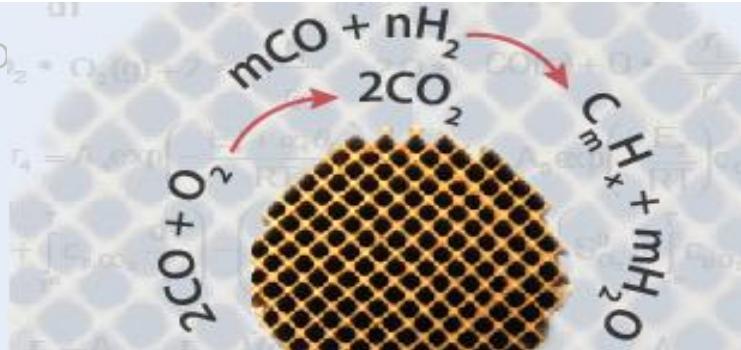
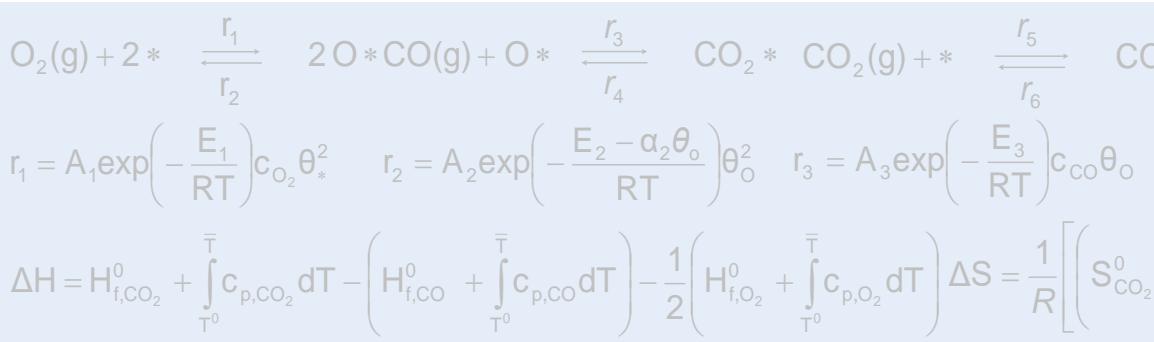


Institute of Energy Process Engineering and Chemical Engineering

Section Chemical Engineering

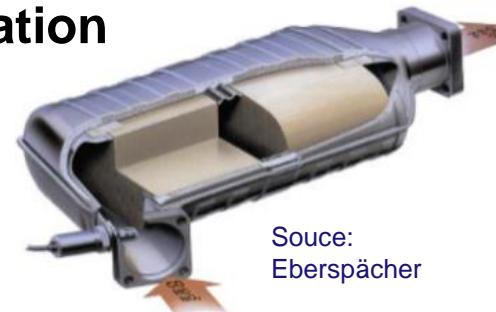
Chair of Reaction Engineering



Sven Kureti

Emission Control / Process Gas Purification

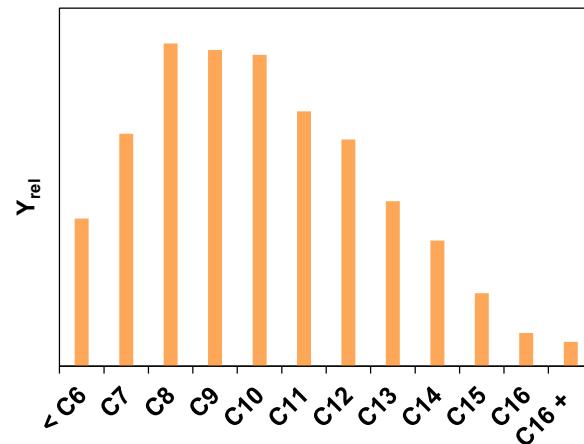
- Oxidation of CO, HC and Soot
- NH₃-SCR, H₂-deNO_x
- NH₃ Oxidation



Source:
Eberspächer

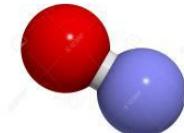
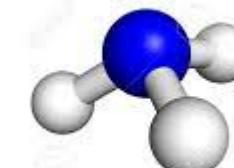
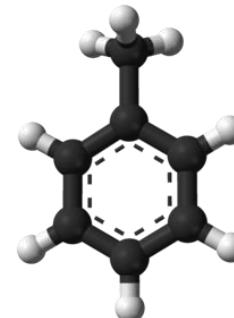
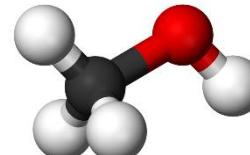
Synthetic and Biogenic Fuels

- FTS, CH₄, MtG
- Olefin Oligomerization
- HVO
- Hydrogenation, Isomerization, Cracking

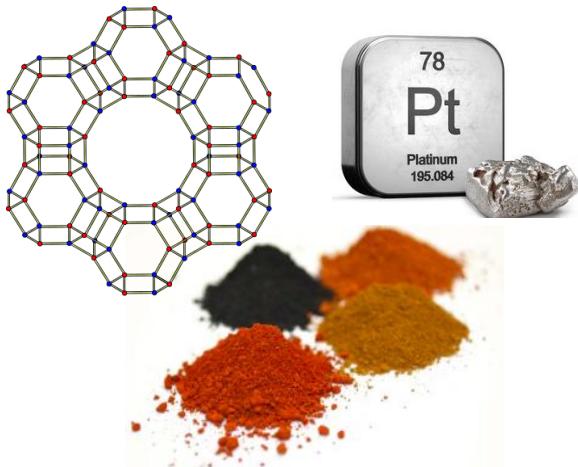


Synthesis of Feedstocks

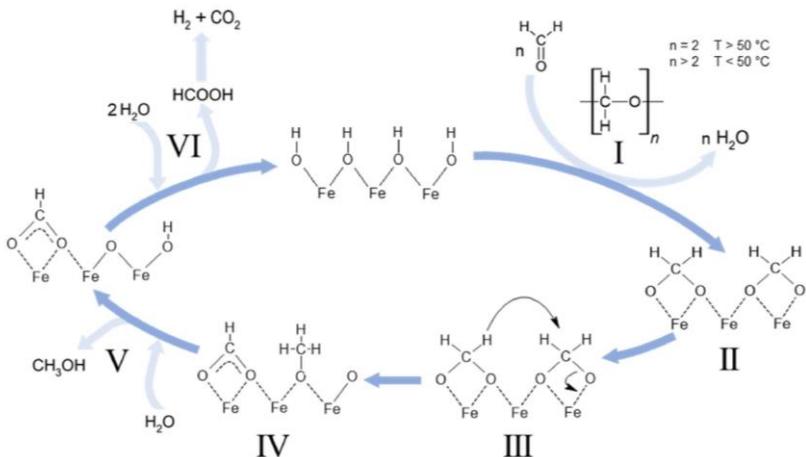
- MtA, MtO
- CH₃OH Synthesis
- NH₃ Synthesis
- NH₃ Combustion



Catalyst Systems



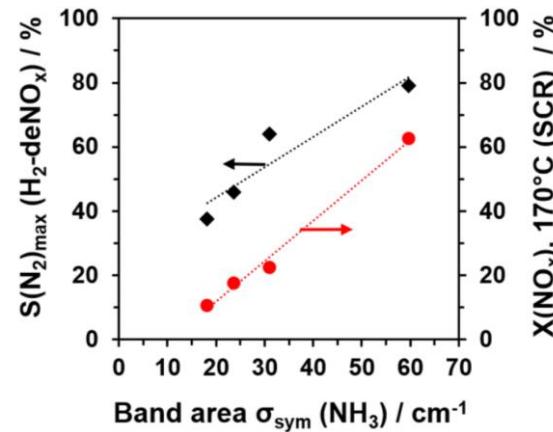
Reaction Mechanisms



Kinetic Modelling

$$\begin{aligned}
 \text{NO(g)} + * &\rightleftharpoons \text{NO*} & r_{13} = A_{13} \exp\left(-\frac{E_{13}}{RT}\right) c_{\text{NO}} \Theta_* & r_{14} = A_{14} \exp\left(-\frac{E_{14}}{RT}\right) \Theta_{\text{NO}} \\
 \text{N}_2\text{O(g)} + * &\rightleftharpoons \text{N}_2\text{O*} & r_{15} = A_{15} \exp\left(-\frac{E_{15}}{RT}\right) c_{\text{N}_2\text{O}} \Theta_* & r_{16} = A_{16} \exp\left(-\frac{E_{16}}{RT}\right) \Theta_{\text{N}_2\text{O}} \\
 2 \text{N*} &\rightleftharpoons \text{N}_2 + 2 * & r_{17} = A_{17} \exp\left(-\frac{E_{17}}{RT}\right) \Theta_{\text{N}}^2 & r_{18} = A_{18} \exp\left(-\frac{E_{18}}{RT}\right) c_{\text{N}_2} \Theta_*^2 \\
 \text{NO*} + * &\rightleftharpoons \text{N*} + \text{O*} & r_{19} = A_{19} \exp\left(-\frac{E_{19}}{RT}\right) \Theta_{\text{NO}} \Theta_* & r_{20} = A_{20} \exp\left(-\frac{E_{20} - \alpha_{20} \Theta_0}{RT}\right) \Theta_{\text{N}} \Theta_0 \\
 \text{N*} + \text{NO*} &\rightleftharpoons \text{N}_2\text{O*} + * & r_{21} = A_{21} \exp\left(-\frac{E_{21}}{RT}\right) \Theta_{\text{NO}} \Theta_{\text{N}} & r_{22} = A_{22} \exp\left(-\frac{E_{22}}{RT}\right) \Theta_{\text{N}_2\text{O}} \Theta_* \\
 \text{NO*} + \text{H*} &\rightleftharpoons \text{N*} + \text{OH*} & r_{23} = A_{23} \exp\left(-\frac{E_{23}}{RT}\right) \Theta_{\text{NO}} \Theta_{\text{H}} & r_{24} = A_{24} \exp\left(-\frac{E_{24}}{RT}\right) \Theta_{\text{OH}} \Theta_{\text{N}}
 \end{aligned}$$

Structure-Activity Relations



→ Fundamentals, targeted catalyst design, process optimization

Kinetic Testing

- Test benches
- Loop Reactor
- NH₃-TPD, HTPD
- FTIR Spectrometers
- Mass Spectrometers
- GC/FID/MS
- Infrared Camera
- Soot Generator

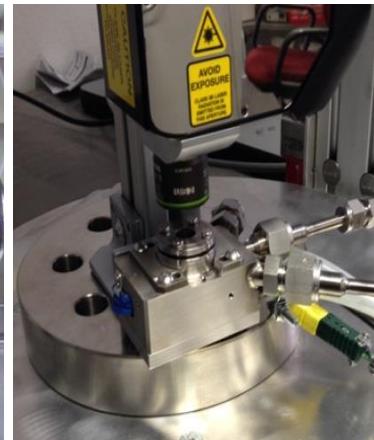


Characterisation

- DRIFTS, FTIR, ATR-IR
- UV-Vis
- Raman with Microscope
- ⁵⁷Fe Moessbauer
- XPS, XRD, XRF
- SEM
- ICP-OES
- Hg Porosimetry, BET

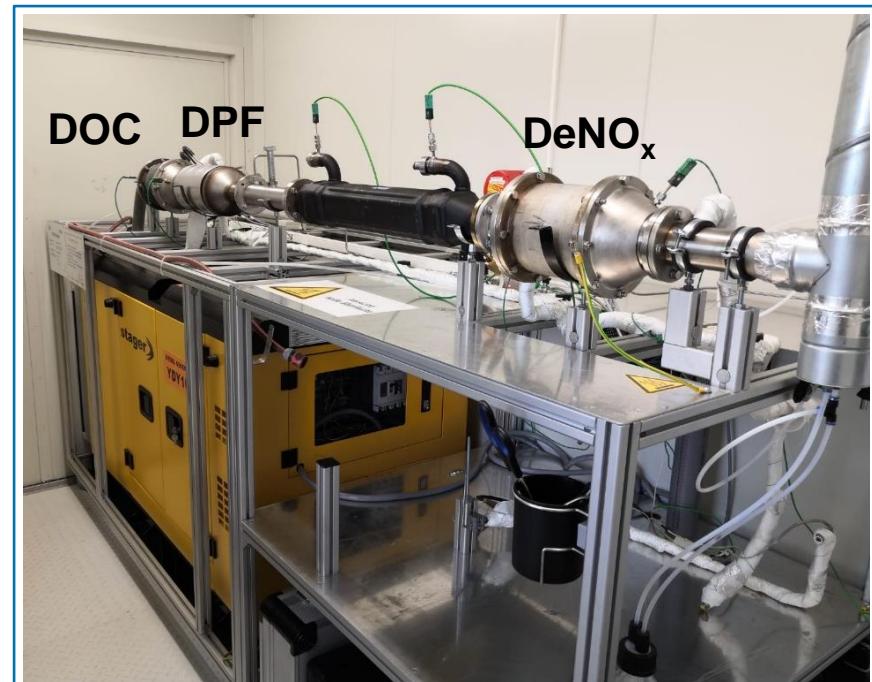
Preparation

- Flame Spray Pyrolysis
- Hydrothermal Synthesis
- Microwave
- Precipitation
- Complexation
- Ceramic Method



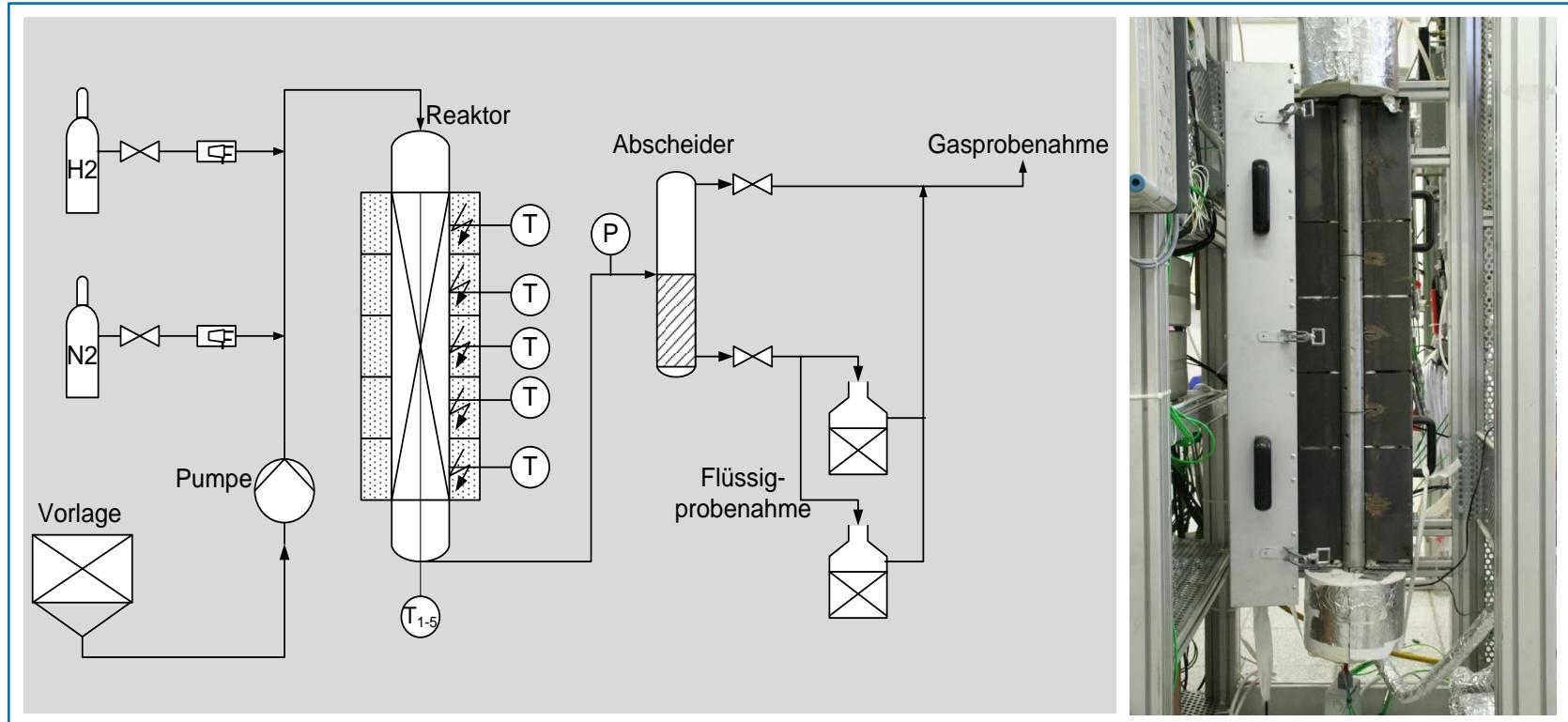
Engine Test Bench

- DI diesel engine (emergency unit)
 - 11 kW at 1500 1/min
 - 3 cylinders, 1532 ccm
 - Compression ratio: 18:1
 - $\lambda = 2 \dots 5$
- Exhaust volume flow:
600...1000 l/min
- Exhaust mass flow:
40...60 kg/h
- Test of real catalysts:
DOC, SCR, H₂-deNO_x,
soot oxidation



Operation Conditions:

- Catalyst Volume: ca. 100 ml
- Pressure: max. 150 bar
- Temperature: max. 400 °C
- LHSV: max. 4 h⁻¹
- Liquid Flow: max. 400 ml/h
- H₂ Flow: max. 300 l/h



- Raw gasoline < 1 L/d
- Catalyst: $m < 60 \text{ g}$ (120 ml)
- SiC dilution of catalyst
- Isothermal fixed-bed reactor
- $T < 750^\circ\text{C}$, $p < 14 \text{ bar}$
- Periphery:
 - Pre-reactor for DME ($\gamma\text{-Al}_2\text{O}_3$)
 - Product separation at 5°C and ambient pressure
 - Continuous monitoring of gas flow
 - Oxidation catalyst for off-gas after-treatment



- R&D using Fe catalysts
- Isothermal fixed-bed reactor
- Automatisierter Betrieb (SPS)
- Specification:
 $T < 500^\circ\text{C}$, $p < 250 \text{ bar}$
- Total flow: max. 1000 ml/min
- Analytics:
Online NDIR spectroscopy for NH₃

