Research Themes (Chemical Processes)

Emission Control / Process Gas Purification

- Oxidation of CO, HC and Soot

- NH_3-SCR, H_2-deNO$_x$
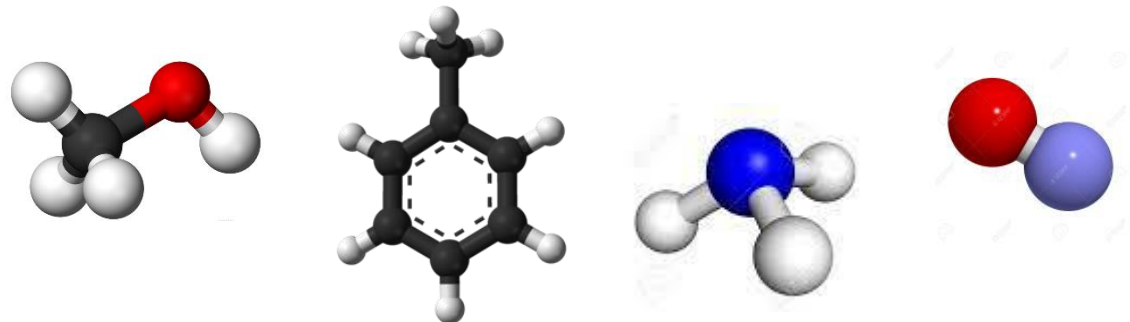
- NH_3 Oxidation

Source: Eberspächer
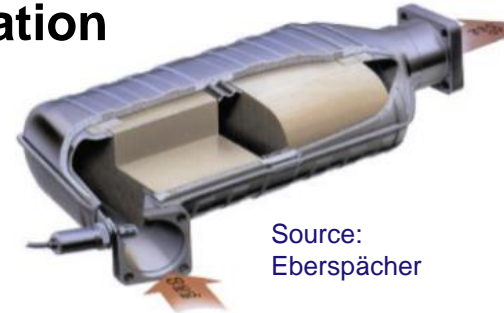
Synthetic and Biogenic Fuels

- FTS, CH_4, MtG

- Olefin Oligomerization

- HVO

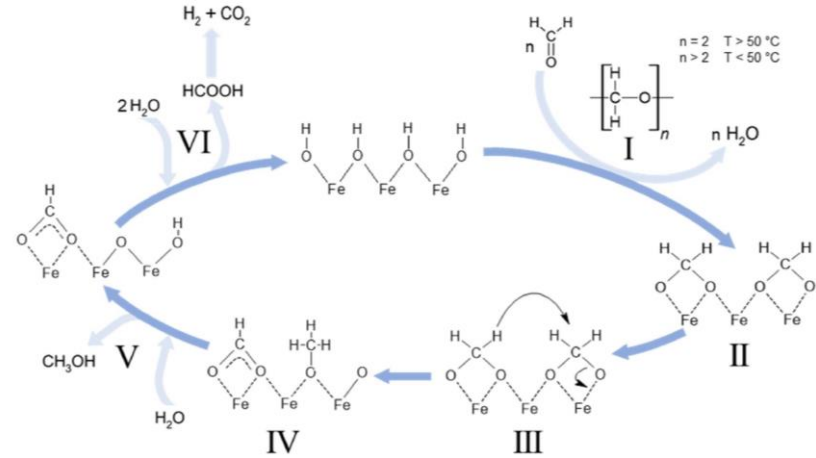- Hydrogenation, Isomerization, Cracking
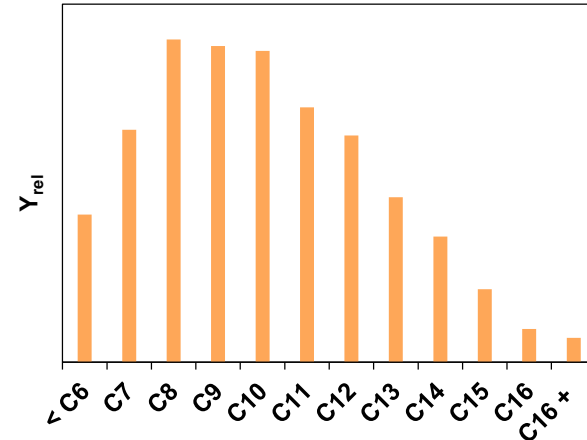
Synthesis of Feedstocks

- MtA, MtO

- CH_3OH Synthesis

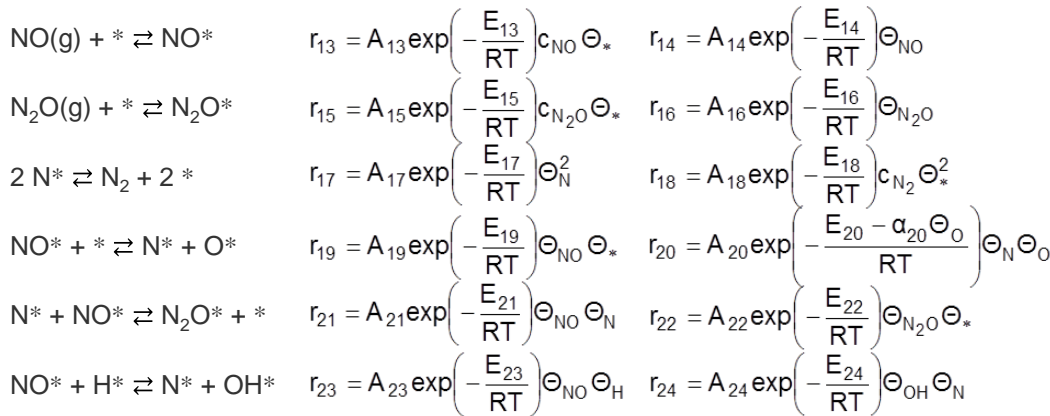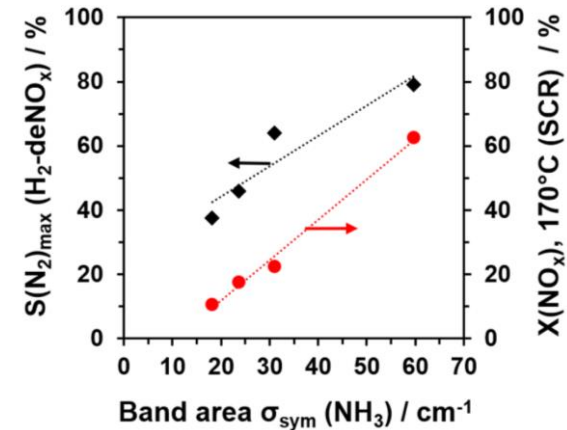- NH_3 Synthesis

- NH_3 Combustion

Catalyst Systems

Reaction Mechanisms

$$H_2 + CO_2$$

$$HCOOH$$

$$2 H_2O$$

VI

V CH_3OH

IV H_2O

III

II

I $n H_2O$

$n = 2 \quad T > 50\,°C$
$n > 2 \quad T < 50\,°C$

Kinetic Modelling

$$NO(g) + * \rightleftarrows NO*$$

$$r_{13} = A_{13}\exp\left(-\frac{E_{13}}{RT}\right)c_{NO}\,\Theta_*$$

$$r_{14} = A_{14}\exp\left(-\frac{E_{14}}{RT}\right)\Theta_{NO}$$

$$N_2O(g) + * \rightleftarrows N_2O*$$

$$r_{15} = A_{15}\exp\left(-\frac{E_{15}}{RT}\right)c_{N_2O}\,\Theta_*$$

$$r_{16} = A_{16}\exp\left(-\frac{E_{16}}{RT}\right)\Theta_{N_2O}$$

$$2\,N* \rightleftarrows N_2 + 2\,*$$

$$r_{17} = A_{17}\exp\left(-\frac{E_{17}}{RT}\right)\Theta_N^2$$

$$r_{18} = A_{18}\exp\left(-\frac{E_{18}}{RT}\right)c_{N_2}\,\Theta_*^2$$

$$NO* + * \rightleftarrows N* + O*$$

$$r_{19} = A_{19}\exp\left(-\frac{E_{19}}{RT}\right)\Theta_{NO}\,\Theta_*$$

$$r_{20} = A_{20}\exp\left(-\frac{E_{20} - \alpha_{20}\Theta_O}{RT}\right)\Theta_N\,\Theta_O$$

$$N* + NO* \rightleftarrows N_2O* + *$$

$$r_{21} = A_{21}\exp\left(-\frac{E_{21}}{RT}\right)\Theta_{NO}\,\Theta_N$$

$$r_{22} = A_{22}\exp\left(-\frac{E_{22}}{RT}\right)\Theta_{N_2O}\,\Theta_*$$

$$NO* + H* \rightleftarrows N* + OH*$$

$$r_{23} = A_{23}\exp\left(-\frac{E_{23}}{RT}\right)\Theta_{NO}\,\Theta_H$$

$$r_{24} = A_{24}\exp\left(-\frac{E_{24}}{RT}\right)\Theta_{OH}\,\Theta_N$$

Structure-Activity Relations

X-axis: Band area σ_{sym} (NH_3) / cm^{-1}

Left Y-axis: $S(N_2)_{max}$ (H_2-deNO$_x$) / %

Right Y-axis: $X(NO_x)$, 170 °C (SCR) / %

→ **Fundamentals, targeted catalyst design, process optimization**

Rational design of Fe catalysts

Characterization of active Fe sites
UV/VIS, TPD, XRD, Mössbauer

Kinetic model

Mechanistic studies
DRIFTS, XANES, SSITKA

Model catalysts

Rational catalyst design

Kinetic studies
CSTR, TPD

Chemical reaction engineering

| deNO$_x$ deN$_2$O | Soot oxidation | CO/HC/NO oxidation | FTS Methanol | CO$_x$ methani-zation |
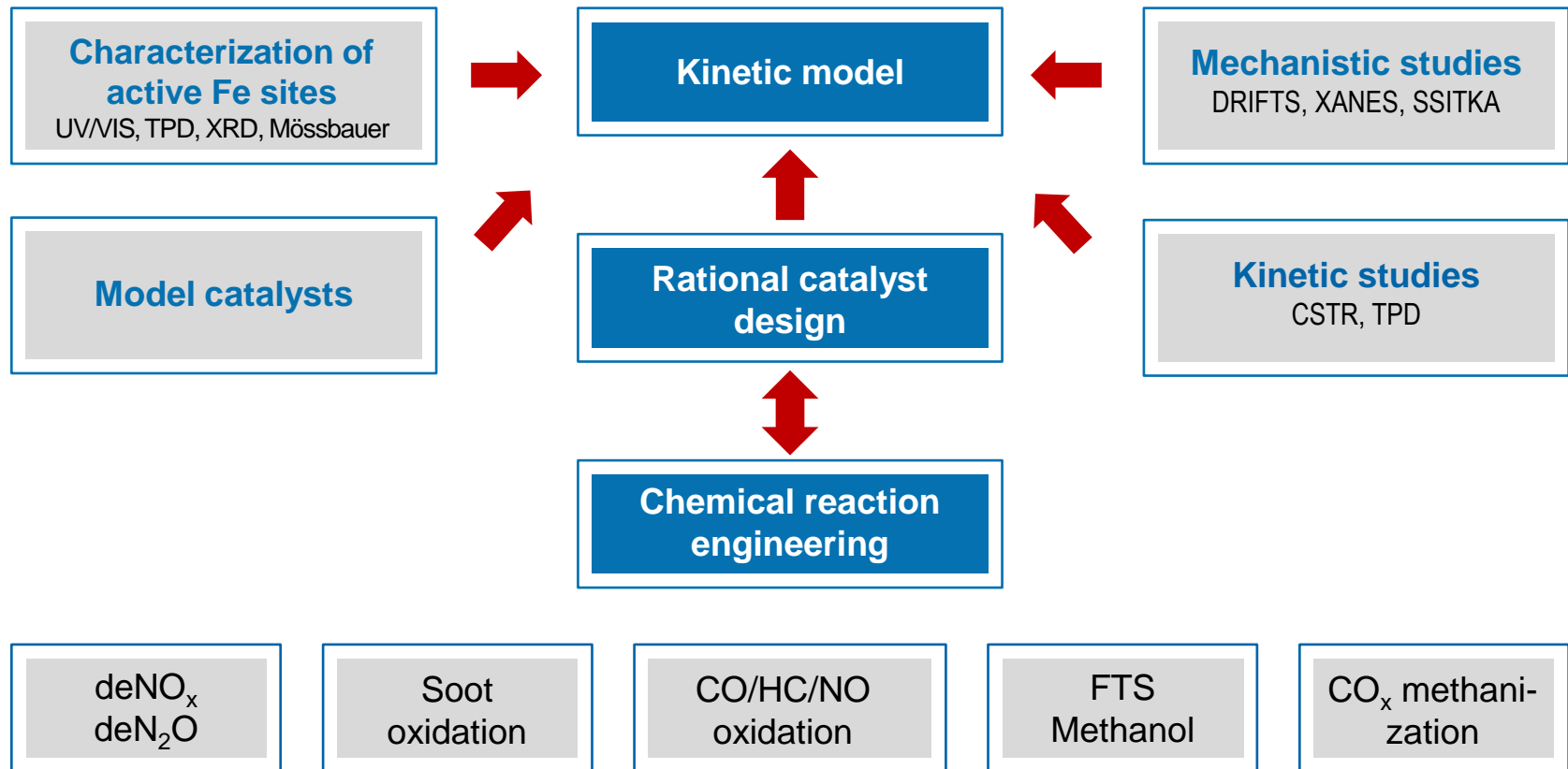
➡ Fundamental understanding of Fe-based catalysts

➡ Novel catalyst concepts

➡ New and optimized processes for material and energy conversion

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