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L-0/L-II | Studies of methanol synthesis by varying reaction parameters

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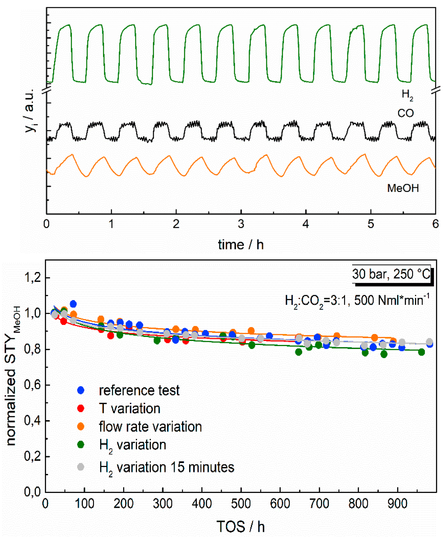
A promising way to benefit from exhaust gases is the conversion of CO_2 into methanol, which is a highly investigated process in industry using the $Cu/ZnO/Al_2O_3$ catalyst [1, 2]. Based on this well-known process, the challenge for using steel mill exhaust gases as raw material is to deal with the impact of dynamic process parameters (p_{gas}, T, p, $\dot{V}$) and the effect of impurities, which could reduce or even prevent an economically sufficient productivity.

1. Experimental – catalyst and setup parameters

- Methanol synthesis was investigated in different setups
- Catalyst used: $Cu/ZnO/Al_2O_3$, provided by Clariant
- Operation modes for testing:
  - temperature range of 170 °C up to 260 °C
  - pressures of 30 bar to 60 bar and
  - feed gas of CO, CO_2, H_2 and N_2 as well as additional gases necessary for testing (e.g. O_2)

3. Dynamic reaction conditions

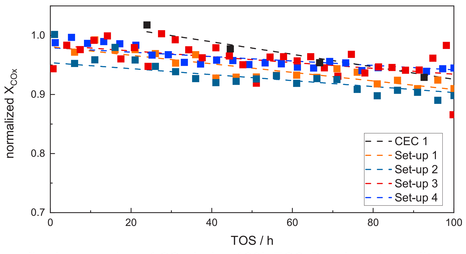
- Making “green” hydrogen usable, renewable resources will cause fluctuations of the supply → intermitting process conditions affect CO_2 hydrogenation activity
- Fluctuating parameters: *T*, $\dot{V}$ and p_{H_2} at 250 °C, 30 bar
- No effect on the overall stability of the catalyst



a) Example of dynamical operation of MeOH synthesis; b) Normalized STY of MeOH during 500 h TOS with intermitting conditions of T, V, p_{H_2} (slow, fast) [3].

2. Benchmark study

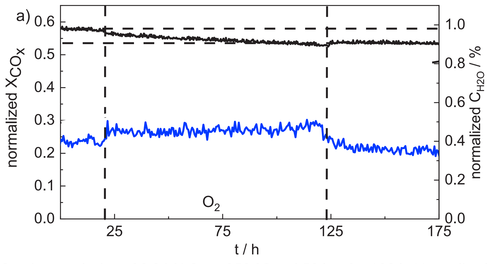
- Performing predefined benchmark for a high comparability
- Equally chosen reaction parameters were monitored over 100 h TOS at 250 °C and 50 bar at given partial pressures
- Normal aging during TOS with a general deviation of X_{CO2} < 3 % leads to consistent data across all setups



Normalized conversion of CO_x during 100h TOS. Benchmark conditions: 250 °C and 50 bar.

4. Deactivation effects of co-feeded O_2

- Limited load of the catalysts with trace substances is required to design necessary purification steps
- Co-feeding impurities while monitoring the activity in methanol synthesis
- O_2 traces act as irreversible (50 bar) catalyst poison on the long-term.



Continuous dosing of 0.06 % O_2 at 250 °C and 50 bar for 108 h. Normalized X_{COx} values (black) and H_2O concentrations (blue) [4].

[1] F. Asinger, *Methanol — Chemie- und Energierohstoff*, Akademie-Verlag, Berlin, 1986.
[2] *Methanol: The Basic Chemical and Energy Feedstock of the Future*, Springer-Verlag, Berlin Heidelberg, 2014.
[3] H. Ruland et al., *ChemCatChem* 2020, 3126.
[4] J. He et al., *Chem. Ing. Tech.* 2020, 1525.

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CO_2 reduction through cross-industrial cooperation between the steel, chemical and energy industries