Catalytic Methanol Synthesis

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Motivation

Challenges: i) Mitigate CO₂ emissions, ii) Store excess renewable energy efficiently

Solution: CO₂ captured at industrial production facilities (cement, coal etc.) and H₂ generated by water electrolysis using excess renewable energy can react and form methanol according to:

\[
\text{CO}_2 + 3 \text{H}_2 \rightarrow \text{CH}_3\text{OH} + \text{H}_2\text{O}
\]

Methanol is produced at industrial scale (~90 million tons/year)¹, because it is a vital chemical feedstock and thus the distribution infrastructure for methanol is well-established. Its energy density is around half of gasoline making methanol applicable for energy storage and transportation².

Cu/ZnO/Al₂O₃ (60/30/10) constitutes the conventional methanol catalyst (200-300°C, 50-100 atm.) with Cu highly influencing the activity, but despite more than 50 years of research, a common agreement on the catalytic active site has not been reached.

Enhanced understanding of Cu-oxide interactions can be beneficial both for the industry and for basic research applications as the principles may be general, and apply to other similar metal-oxide catalysts.

Methods


Results

Preliminary quantitative TPD experiments show simultaneous peak H₂ and CO₂ desorption at ~140-170°C, which studies have attributed to desorption of HCOO from Cu₆. However, the desorption profiles are complicated by contributions from the oxide.

The STY (space time yield) to Cu surface area relation for different catalysts indicate an electron support effect influencing the STY in addition to the Cu surface area.

Conclusions and Further Work

- Quantitative evaluation of surface species coverages at operational conditions can be conducted by rapid cooling with N₂.

- STY vs. Cu surface area indicates a support effect potentially due to electronic transfer phenomena

- Preliminary results indicate a strong influence of \( \theta_{\text{HCOO}} \) on TOF

- Future DRIFTS studies are designed to relate concurrent CO₂ and H₂ desorption at a specific temperature interval to Cu-HCOO desorption

- Blank experiments may allow subtraction of the contributions from the oxides to the CO₂, CO, and H₂ desorption profiles thus simplifying the quantitative analysis of the Cu-HCOO desorption

References

6. Nielsena†, A. D. Jensena, and J. M. Christensena*

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Experimental Setups

Flow reactor setup applications:

- Methanol activity by GC
- Catalyst cooling before quantification of surface species with MS by TPD
- Estimate qualitatively the desorption temperatures of surface species by DRIFTS

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