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CO2UTIL

Towards utilization of CO_2 as a green and versatile commodity chemical: Clean synthesis of Methanol and Dimethyl Carbonate

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Background

- For two centuries, human beings have been transferring carbon from the lithosphere to the atmosphere
- The boundary separating the truly dangerous consequences of emissions from the merely unwise is probably located near, but below a doubling of concentrations of CO_2 that was in the atmosphere before the Industrial Revolution (~280 ppmv)
- Presently, the world's coal-, oil- and natural gas industries dig and pump up about seven billion tons of carbon a year
- Over the past 30 years, as the world production of goods and services grew at 3% a year, while carbon emissions rose half as fast
- For global emissions to be the same in 2056 as today, the carbon intensity will need to fall as fast as the global economy grows
- Holding CO_2 emissions constant for 50 years without compromising economic growth is a challenge!
- It can, however, be achieved by the combination of efficiency gains, renewable energy and CO_2 utilization.

Ref.: Socolow & Pacala: A plan to keep carbon in check. SciAm 295(3): 28-35

Project aims

- Developing green chemical products via a sustainable process in accordance with Green Chemistry principles
- Synthesis of methanol and DMC using CO_2
  - Value enhancement of a secondary resource from anthropogenic source
- The conventional method for methanol production is based on fossil feedstock and the production of DMC involves the use of toxic phosgene or CO
  - Reduction of the hazard from solvents and chemicals
  - Explore safe and environmentally sound reaction routes and energy-efficient processes
  - Identify new, effective catalysts for methanol and DMC syntheses
- Develop a dynamic simulation system that can be used in studying the realization of different process routes from process control viewpoint

Consortium members

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Reforming

- Process for producing synthesis gas (H_2 + CO)
- Synthesis gas is an important raw material in many chemical synthesis (e.g. methanol synthesis)
- Synthesis gas can be produced from almost any carbon source ranging from natural gas to biomass
- CO_2 is used as a feedstock in *dry reforming*
- Reaction
  - $CO_2 + CH_4 \leftrightarrow 2H_2 + 2CO$
- Challenges:
  - sufficient conversion → high temperature is needed
  - carbon formation problem → catalyst resistive of carbon is needed
- Research focus:
  - catalyst development and optimization
  - reaction conditions optimization

Methanol synthesis

- Methanol is an important product and feedstock in chemical industry
- Commercially methanol is produced from synthesis gas

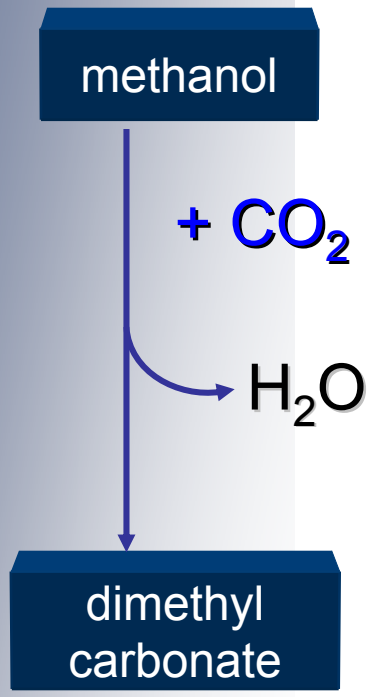
$$CO + 2H_2 \leftrightarrow CH_3OH$$

- It is possible to use CO_2 as a feedstock in methanol synthesis

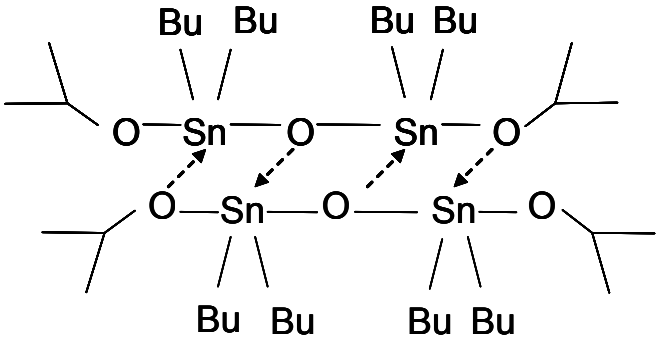
$$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O$$

- Challenges
  - reaction is thermodynamically unfavorable
  - more active catalysts are needed
    - » catalyst development and optimization

Use of homogeneous catalysts



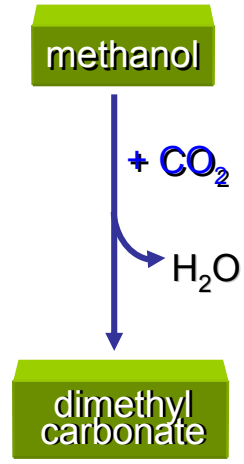
- Utilization of secondary CO_2 in methanol and dialkyl carbonate production over heterogeneous and homogeneous catalysts
- Direct synthesis of dimethyl carbonate (DMC) using carbon dioxide as solvent and reagent for its fixation to methanol
- Water, the co-product of the reaction reversibly poisons the active centers.



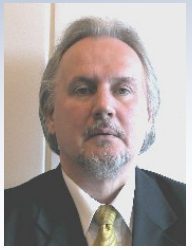
Green Chemistry

- Waste prevention
- Atom economy
- Harmless solvents
- Minimizing energy use
- Renewable feedstock
- Catalytic reagents
- Safe processes

	atom economy
ethylene carbonate + methanol	59 wt%
urea + methanol	72 wt%
carbon dioxide + methanol	83 wt%



Dynamic simulations



- Dynamic simulations will be prepared for the whole reaction chain, from secondary CO_2 to different products such as synthesis gas, methanol and DMC.
- The dynamics of different process alternatives and variants for processing routes will be considered.
- This will give insight for possibilities to manage and optimize production chains.
- Finally, the potential combination of sequential reaction steps from CO_2 and H_2 to MeOH and DMC, offers an ultimate pathway to an optimized process.

International collaboration within the project

- Green route to DMC
- DMC production in supercritical conditions
- Innovative synthesis routes to ionic liquids and applications
- Researcher exchange is planned to foster knowledge production for new milestones

Summary

- The results will improve on the technologies aiming at recovery and utilization of secondary CO_2
- Implementing Green Chemistry and Engineering improves the environmental impacts of chemical products and processes while also offering economic incentives
- The proposed scientific methodology is knowledge-driven and benefits from the academic expertises of the Finnish and French research groups
  - catalysis
  - kinetics
  - process engineering
  - environmental engineering
  - organometallic chemistry