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Integrated CO₂ capture and conversion to formic acid/methanol via methyl formate

Aim

The aim of this project is to evaluate an integrated route for CO₂ capture and formic acid/methanol production via methyl formate.

Justification

Carbon Capture and Utilization (CCU) has been recognized as one of the most promising technologies for mitigating climate change due to its capacity for large-scale CO₂ reduction. The main challenge of these technologies is that a large amount of thermal energy must be provided to supply high-purity CO₂ and purify the product¹. An approach to eliminate the CO₂-desorption cost is to integrate CO₂ capture and conversion (ICCU).

ICCU strategies have been proposed for the production of formic acid (FA)/formates, methanol (MeOH), urea, methyl formate (MeF), carbonates, syngas, and materials suitable for construction². FA, MeOH, and MeF are particularly interesting molecules for the research conducted in our group. FA and MeOH can be used directly as fuels, are important feedstocks for the chemical industry, and became recently attractive energy carriers. MeF can also be used to produce several industrially important chemicals, and by a simple hydrolysis reaction can generate simultaneously FA and MeOH³.

Both FA and MeOH production from CO₂ have been thoroughly investigated. CO₂ hydrogenation to FA is thermodynamically unfavourable in the gas phase. Often, FA is stabilized in the form of formate adducts by reaction with a base. The isolation of pure FA from the stabilizing reaction media is consequently one of the major challenges in process schemes for CO₂-based FA production⁴. Regarding CO₂ hydrogenation to MeOH, the challenge relies on equilibrium limitations at high reaction temperatures and pressures, and the limited availability of catalysts capable of efficiently catalyzing the reaction under mild conditions⁵. A route for the production of FA and/or MeOH from CO₂ via MeF could be an alternative to sidestep these challenges.

In this project, an ICCU strategy for the integrated capture and conversion of CO₂ to MeF will be evaluated, as well as the potential for FA/MeOH production from the generated MeF (Figure 1). The CO₂ needed to produce MeF will be absorbed by MeOH. Then, the mixture of CO₂ and MeOH, together with H₂ will be used to synthesize MeF. The possibility to hydrolyse the purified MeF to FA or further hydrogenation to MeOH will be investigated.

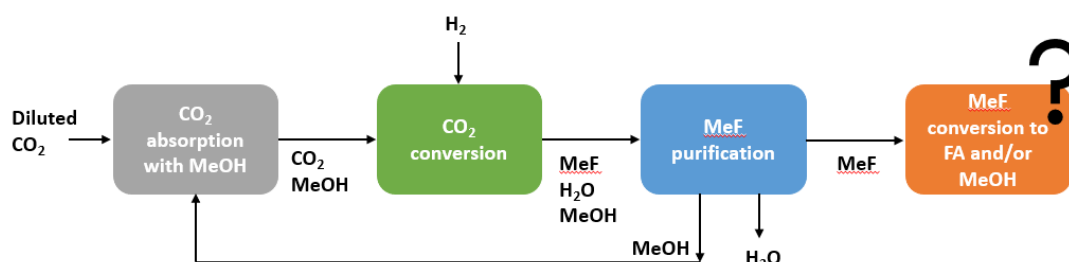


Figure 1. Integrated CO₂ capture and conversion to FA/MeOH via MeF process scheme.

Program

1. Literature study on the main steps of the process.
2. Selection of the unit operations and the models to use.
3. Process modeling using ASPEN.

References

1. K. M. G. Langie, K. Tak, C. Kim, H. W. Lee, K. Park, D. Kim, W. Jung, C. W. Lee, H.-S. Oh, D. K. Lee, J. H. Koh, B. K. Min, D. H. Won and U. Lee, *Nature Communications*, 2022, **13**, 7482.
2. C. M. Jens, L. Müller, K. Leonhard and A. Bardow, *ACS Sustainable Chemistry & Engineering*, 2019, **7**, 12270-12280.
3. J. J. Corral-Pérez, A. Bansode, C. S. Praveen, A. Kokalj, H. Reymond, A. Comas-Vives, J. VandeVondele, C. Copéret, P. R. von Rohr and A. Urakawa, *Journal of the American Chemical Society*, 2018, **140**, 13884-13891.
4. C. M. Jens, M. Scott, B. Liebergesell, C. G. Westhues, P. Schäfer, G. Franciò, K. Leonhard, W. Leitner and A. Bardow, *Advanced Synthesis & Catalysis*, 2019, **361**, 307-316.
5. C. A. Huff and M. S. Sanford, *Journal of the American Chemical Society*, 2011, **133**, 18122-18125.