Computer Aided Process Engineering

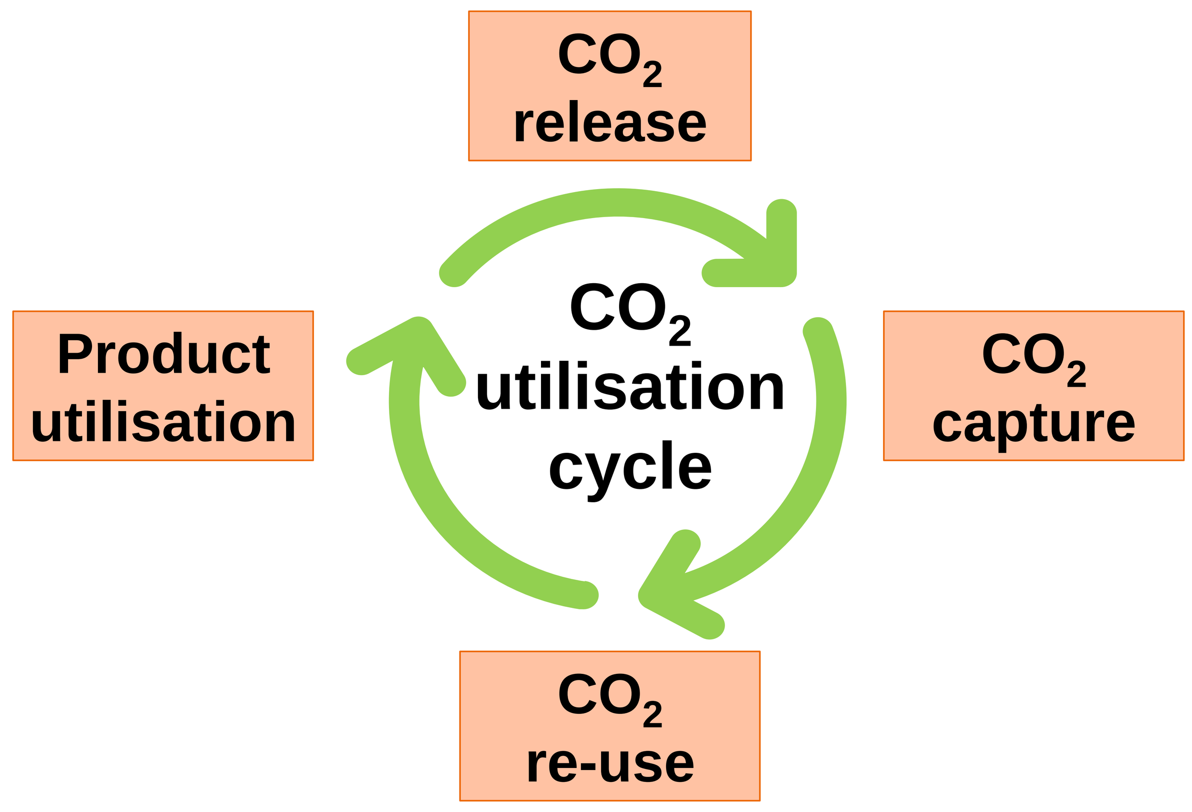
Direct Dimethyl Carbonate Production from Carbon Dioxide and Methanol

A. Rouxhet, L. Baggio, M. Govaert, B. Marchal, G. Léonard

Université de Liège, Department of Chemical Engineering – PEPs www.chemeng.uliege.be

Introduction

The world we live in is largely carbon-based, the society's defossilisation is thus a more rational objective than its decarbonisation. In this framework, it is possible to synthesise dimethyl carbonate (DMC) from captured CO_2 and methanol. DMC production is appealing as it is generally considered as a green chemical (non-toxic, biodegradable,…), which can replace toxic phosgene in polycarbonate synthesis. Two alternative processes, which differ in the employed dehydrating agent, are explored in this work. Indeed, DMC synthesis is an equilibrium-limited reaction yielding water as a by-product. Dehydrating the system enables to shift the equilibrium. One process uses 2-cyanopyridine (2-CP) as the dehydrating agent, while the other employs ethylene oxide (EO). Both options are compared based on their techno-economic assessment.

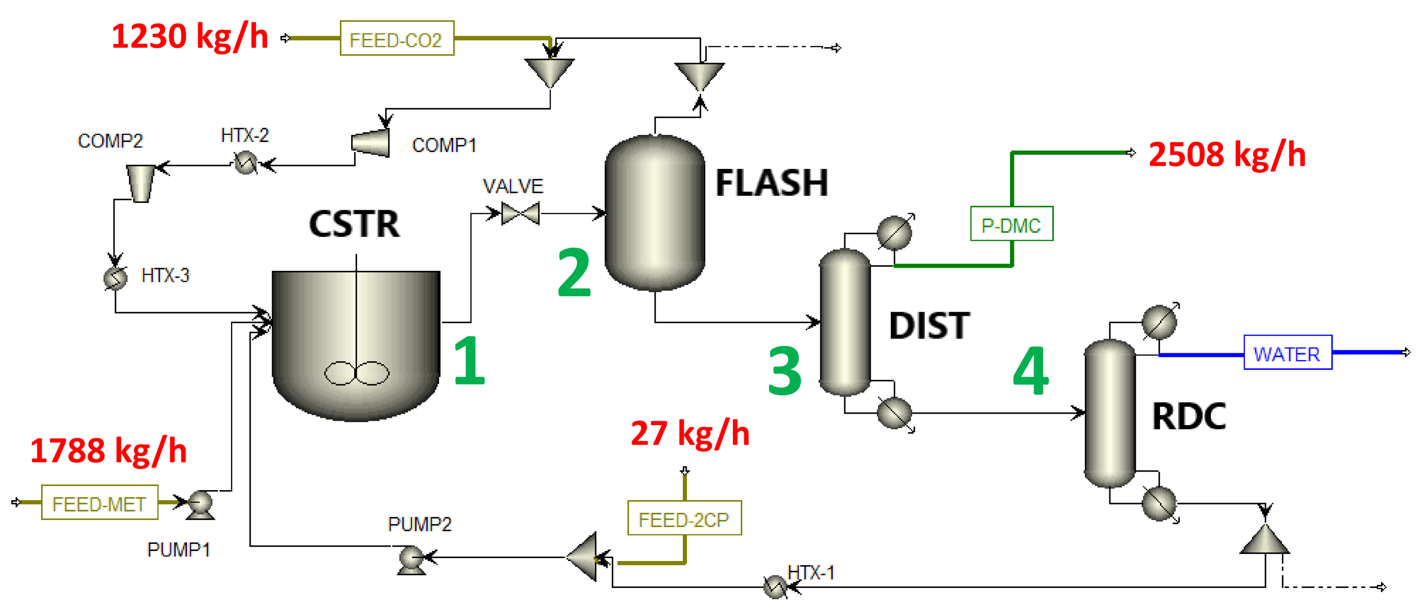


Process design

2-CP process

$$CO_2 + CH_3OH \Leftrightarrow (CH_3O)_2CO + H_2O$$

$$H_2O + 2\text{-}CP \Leftrightarrow 2\text{-}PA$$

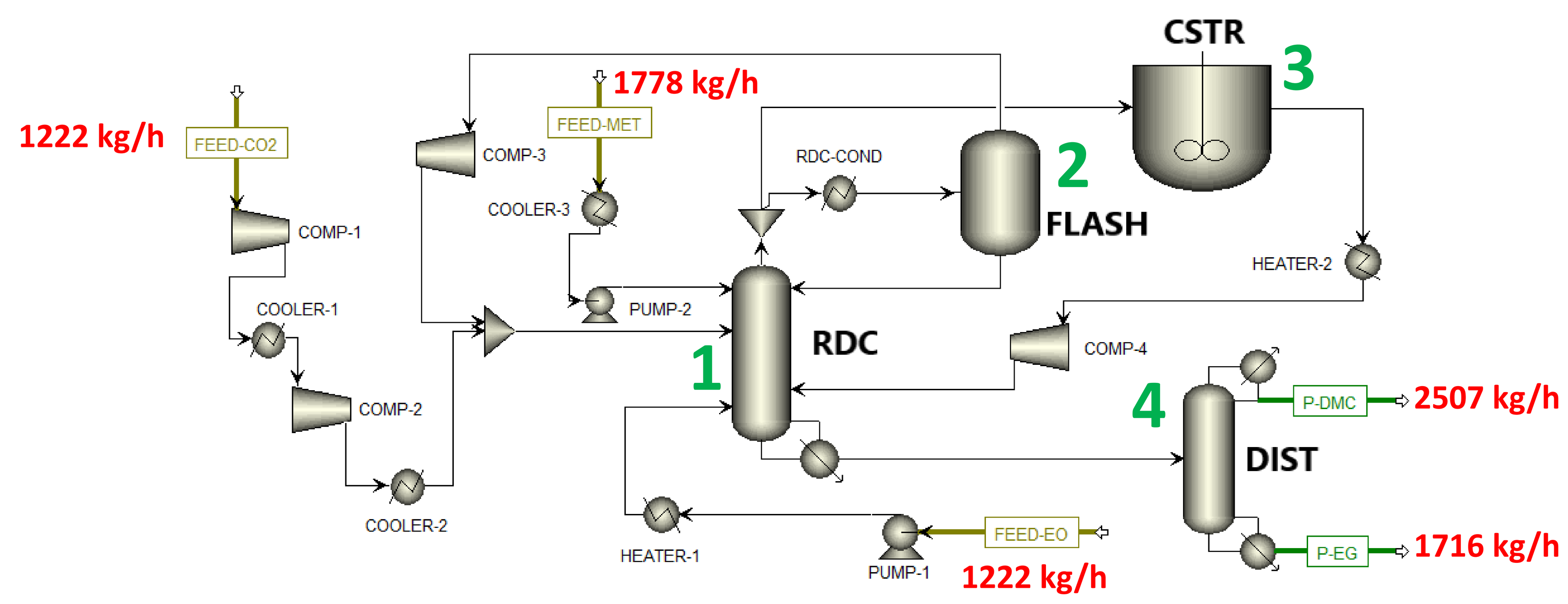


1. CSTR at 120°C and 30 bar
2. Flash separation at 1 bar: recovering of unreacted reagents
3. Distillation at 1 bar: purification of final product (99.8 wt-%)
4. Reactive distillation at 1 bar: transformation of 2-picolinamide (2-PA) back in 2-CP

EO process

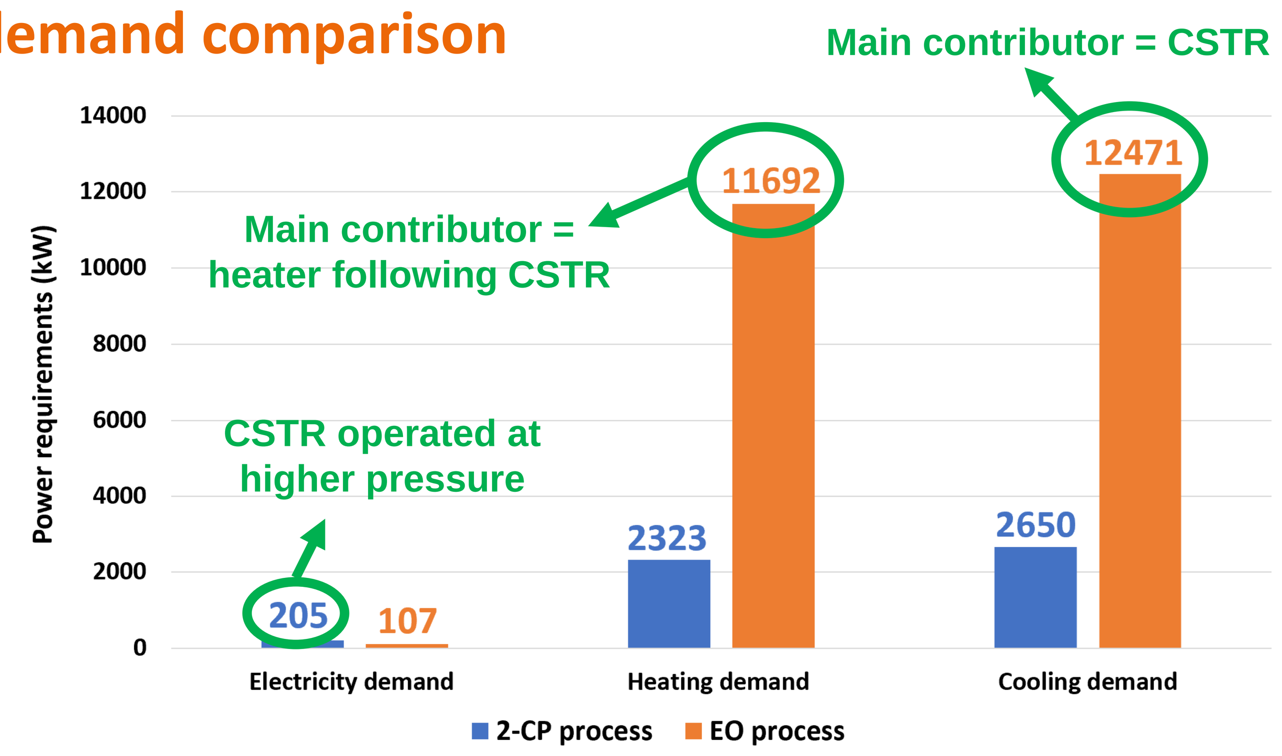
$$CO_2 + CH_3OH \Leftrightarrow (CH_3O)_2CO + H_2O$$

$$H_2O + EO \rightarrow EG$$

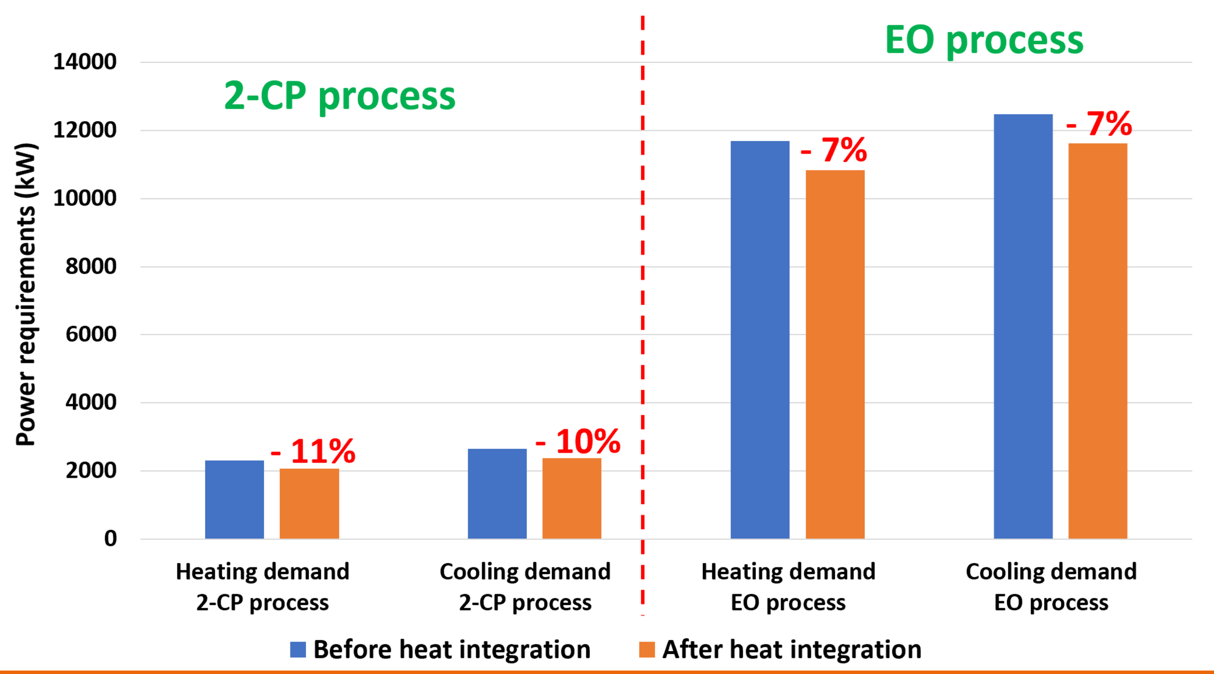


1. Reactive distillation at 15 bar: formation of ethylene glycol (EG)
2. Flash separation at 15 bar: recovering of unreacted reagents
3. CSTR at 114°C and 15 bar
4. Distillation at 1 bar: purification of final products (DMC at 99.7 wt-% and EG at 99.9 wt-%)

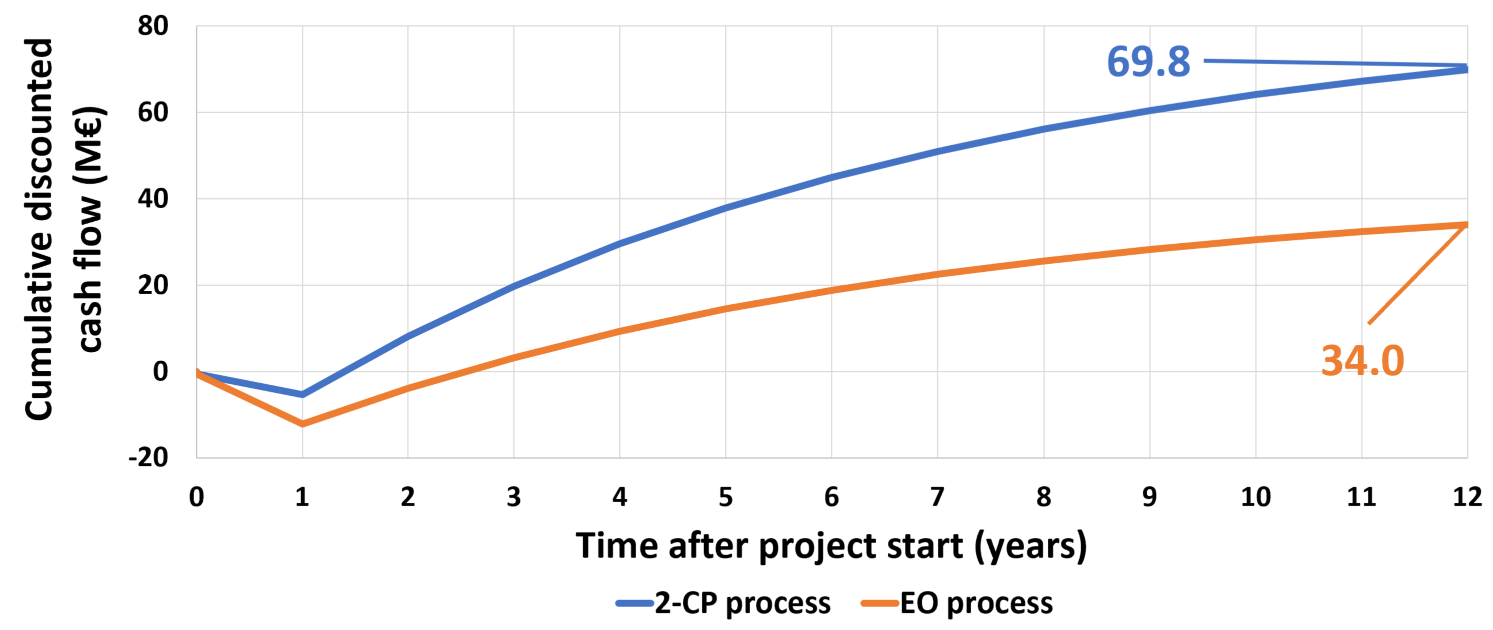
Energy demand comparison

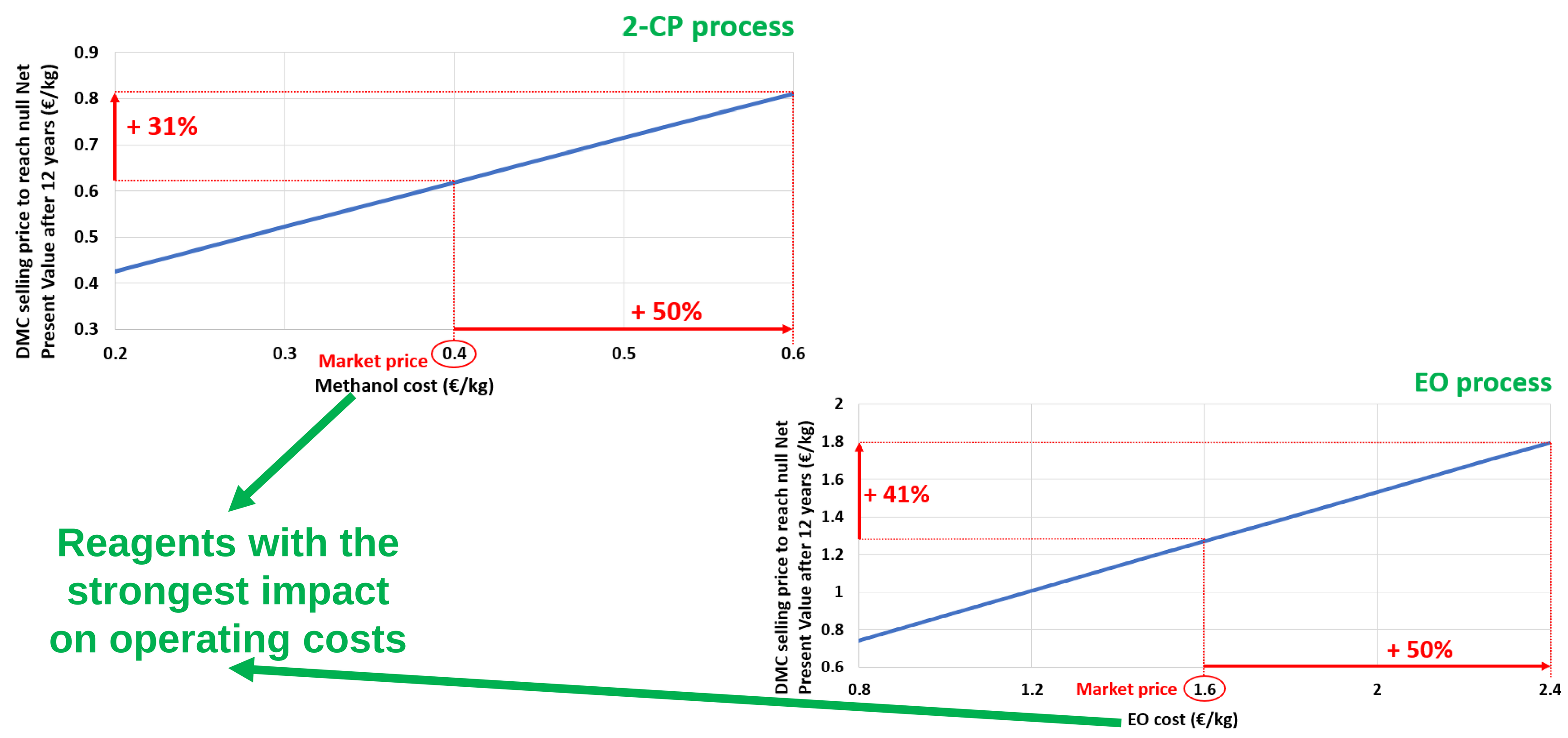


Potential energy savings through heat integration



Economical analysis





Conclusion

Based on these results, producing DMC from non-fossil-based reagents seems feasible. The best option for the dehydrating agent used to shift the reaction equilibrium is 2-CP, both from economic and energetic points of view. However, the results should be refined with better optimisation of both processes, especially in terms of design options. The production of sustainable methanol from captured CO_2 and green H_2 was also investigated and showed the need for low-price renewable energy to ensure the process viability based on sustainable energy sources. Finally, the heat integration analysis should be updated for the possible interactions between the DMC and methanol production units.