

Experimental study of catalysts and process designs for chemical synthesis using H₂ and CO₂





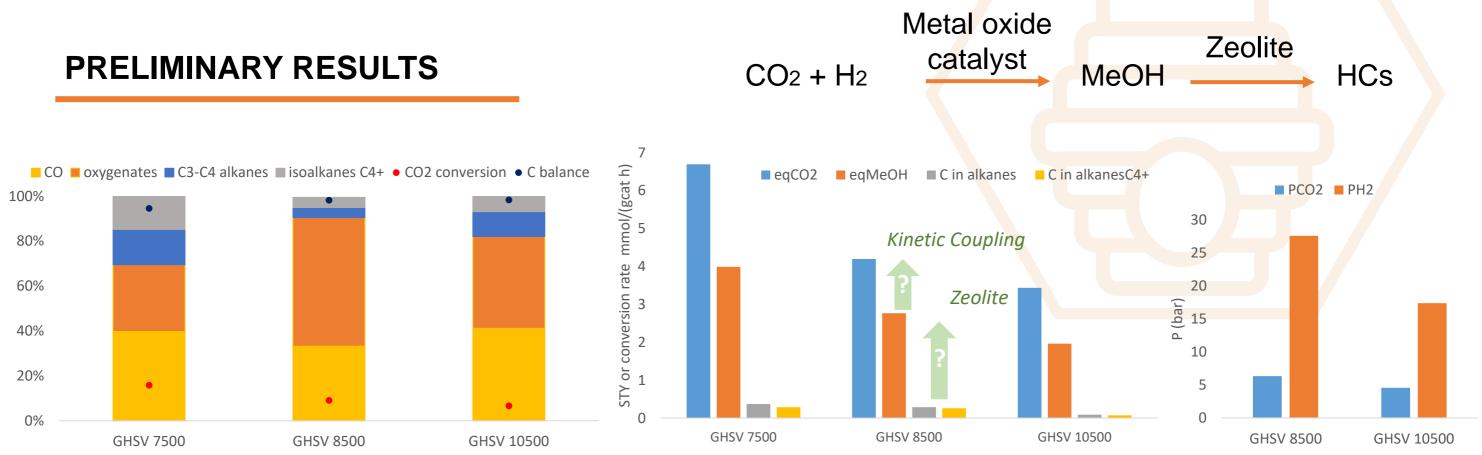
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INTRODUCTION

Carbon neutral fuels are getting more and more attractive due to the global warming and energy crisis. The main goal of this project is to produce green added-value fuels (e.g. jet, higher length hydrocarbons) directly from CO₂ and H₂ in a **one-step reaction**.

Until today this process has been studied mainly using syngas (CO/H₂) as a feed and producing hydrocarbons through the Fischer-Tropsch Synthesis route, especially for certain ranges of hydrocarbon numbers(3,5,7).

The idea is to use CO_2 and H_2 feeds via methanol as intermediate by combining the CO_2 to methanol process on reducible oxide catalysts with the wellknown **Methanol to Hydrocarbons** chemistry. The latter will be modified through new catalyst development to selectively produce gasoline-range hydrocarbons.



Effect of different Gas Hourly Space Velocities (ml/gcat/h) on (a) product distribution, conversion and carbon balance, (b) space time yields of equivalent CO2 and MeOH and alkanes produced, (c) partial pressure or reactants

Fixed bed reactor, Catalyst: InCo + BEA Si/Al 19 (1:1) mixed bed configuration, $T = 300^{\circ}C$, P = 40 bar, $GHSV_{CO2} = 1500 \text{ ml}_{CO2} \text{ g}_{cat}^{-1} \text{ h}^{-1}$

OBJECTIVES

- Development of new catalytic materials(1,2,4,8) and large-pores zeolites (6)
- Catalyst screening, esp. zeolites not tested for MTH in high CO₂ pressures / H₂ environments
- Target in high C4+ selectivity (at high C balances)
- Scale up for best materials in semi-pilot scale reactor
- Study and optimize process conditions

REFERENCES

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- 1. Wang, J. et al. A highly selective and stable ZnO-ZrO2 solid solution catalyst for CO2 hydrogenation to methanol. Sci. Adv. 3, 1–11 (2017).
- 2. Ruddy, D. A. et al. Methanol to high-octane gasoline within a market-responsive biorefinery concept enabled by catalysis. Nat. Catal. 2, 632–640 (2019).
- 3. Zhang, Q., Li, X., Asami, K., Asaoka, S. & Fujimoto, K. Synthesis of LPG from synthesis gas. Fuel Process. Technol. 85, 1139–1150 (2004).
- 4. Dokania, A. et al. Designing a Multifunctional Catalyst for the Direct Production of Gasoline-Range Isoparaffins from CO 2. JACS Au 1, 1961–1974 (2021).
- 5. Léonard, G., Giulini, D. & Villarreal-Singer, D. Design and Evaluation of a High-Density Energy Storage Route with CO2 Re-Use, Water Electrolysis and Methanol Synthesis. Computer Aided Chemical Engineering vol. 38 (2016).

- 7. Morales, A. & Leonard, G. Simulation of a Fischer-Tropsch reactor for jet fuel production using Aspen Custom Modeler. Computer Aided Chemical Engineering 22, 301-306 (2022).
- 8. Martín, N. et al. MOF-derived/zeolite hybrid catalyst for the production of light olefins from CO2. ChemCatChem 12, 5750–5758 (2020)

^{6.} Li, C., Yuan, X. & Fujimoto, K. Direct synthesis of LPG from carbon dioxide over hybrid catalysts comprising modified methanol synthesis catalyst and β-type zeolite. *Appl. Catal. A Gen.* **475**, 155–160 (2014).