Power to Fuels

Modelling of methanol production

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Energy Transition

- Electricity production
- Storages
- Heat production
- Mobility
- Systems
- Business
- Materials
Where do we need power t X?

PtX - Carbon compounds/H₂
Methanol: a clean-burning multipurpose fuel

Sources: Methanex, Investor Presentation, March 2019
ATA Markets Intelligence S.L., Renewable Methanol Report, December 2018

Emission reductions when compared to heavy fuel oil

Sources: Methanex, Investor Presentation, March 2019
ATA Markets Intelligence S.L., Renewable Methanol Report, December 2018

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Renewable methanol production

Source: ATA Markets Intelligence S.L., Renewable Methanol Report, December 2018

Source: The Methanol Institute and Qafiq
Full system modelling
Aspen Plus
Methanol plant
Study boundaries

Process simulation

Economic feasibility

Nyári et al. 2020 J. CO₂ utilization,
https://doi.org/10.1016/j.jcou.2020.101166
Production cost of methanol

Bottlenecks of economic viability

- Electricity cost (20 - 40 €/MWh)
- CO2 cost (25 - 75 €/t)
- O2 selling (Yes - No)
- Scale of plant (250 - 10 kt/a)

Levelised cost of methanol (€/ton)

Comparison to other LCOMeOH studies

This paper
Asif et al., 2018
Atsonios et al., 2016
Hannula, 2015a
Kourkoumpas et al., 2016
Pérez-Fortes et al., 2014
Rivera-Tinoco et al., 2016
Szima and Cormos, 2018
Tremel et al., 2015
Varone and Ferrari, 2015
Wiesberg et al., 2016

Reactor modelling
Computational Fluid Dynamics (CFD)
Computational Fluid Dynamics

CFD modelling of multi-tubular and milli-scale reactors.

**Aim and objectives**
Development of intensified cost-effective methanol synthesis process starting from $\text{H}_2$ and $\text{CO}_2$ using modular milli-scale reactor design.

Adiabatic and Isothermal reactors

Software: OpenFOAM  
Izbassarov *et al.* (2021)  
[https://doi.org/10.1016/j.ijhydene.2021.02.031](https://doi.org/10.1016/j.ijhydene.2021.02.031)
2D Fixed-bed Reactor

Adiabatic reactor

\[ T_i = 523K, p_i = 5MPa, Re = 100, SV = 6 \text{ m}^3/\text{kg}_{\text{cat}} \text{ h} \]

Izbassarov et al (2021)

https://doi.org/10.1016/j.ijhydene.2021.02.031
2D Fixed-bed Reactor

Adiabatic

 Isothermal

Izbassarov et al (2021)
https://doi.org/10.1016/j.ijhydene.2021.02.031

p2xenable.fi
Experimental studies

Lab-scale methanol synthesis reactor
Experimental reactor system

Methanol synthesis from CO\textsubscript{2} and H\textsubscript{2}

Process conditions
T: 200 – 250 °C
p: 30 – 50 bar

Commercial
Cu-based catalyst

Optimized with modelling
Reactor Details

Height: 50 cm
Inner diameter: 3,8 cm
(Volume: 0.567 L)

Integrated oil cooling channels on the outside
3 places for temperature sensors
3 places for pressure sensors
Research topics

- Different catalyst materials
- Different catalyst packings
- Different feed gas compositions (e.g. CCU product gases)
- Validation of simulation results (Aspen Plus & OpenFoam simulation)
- The effect of operating conditions in modified cases
Conclusion

Methanol is a versatile chemical compound that can be implemented into the current fuel infrastructure.

Technically viable to synthesise from CO₂ and H₂.

Price of H₂ is significant contributor to high methanol production cost.

Efficiency improvements needed.