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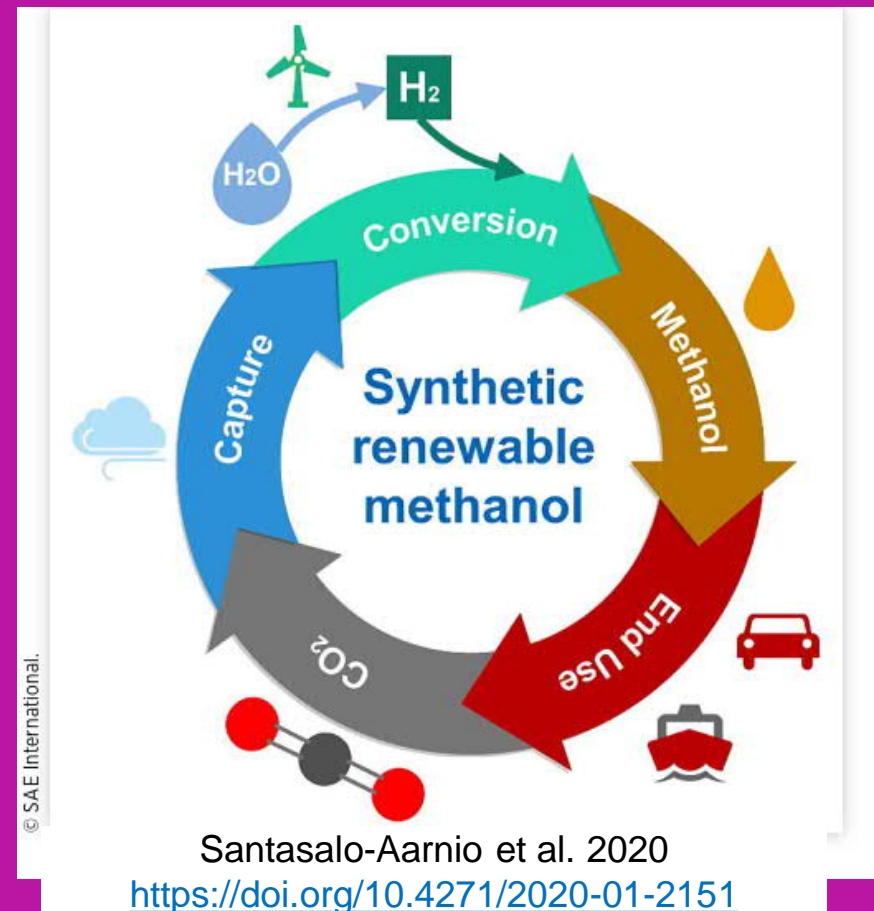
Aalto University
School of Engineering

Power to Fuels

Modelling of methanol production

*Annikka Santasalo-Aarnio
Judít Nyári, Markus Laitinen*

Daulet Izbassarov, prof. Ville Vuorinen



*Aalto University
Energy Conversion
Department of Mechanical Engineering*

Research Group of Energy Conversion

Aalto University

Head
Prof. Martti Larmi



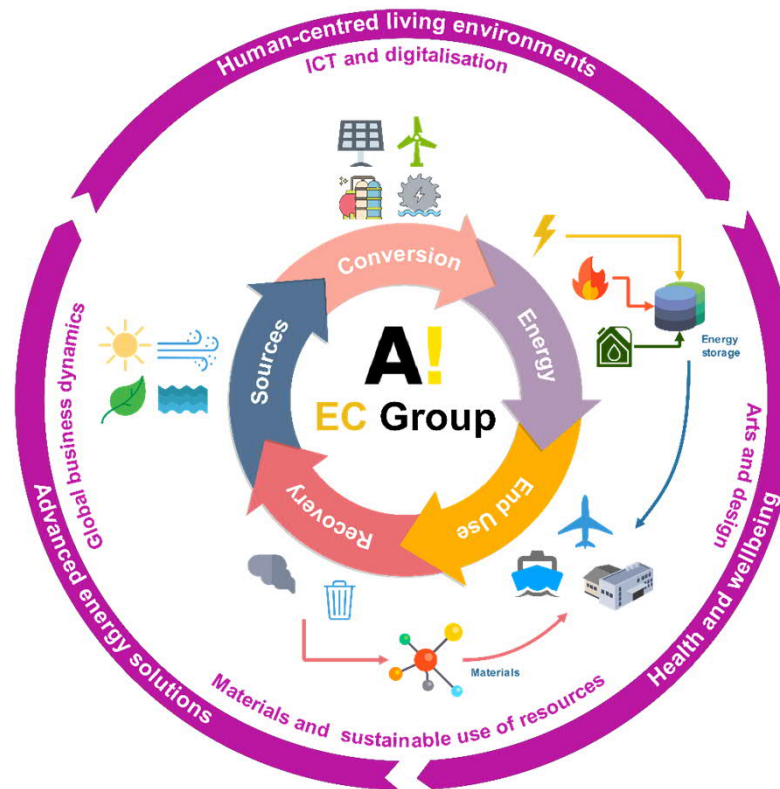
Prof. Annukka Santasalo-Aarnio



Prof. Ville Vuorinen



Prof. Mika Järvinen



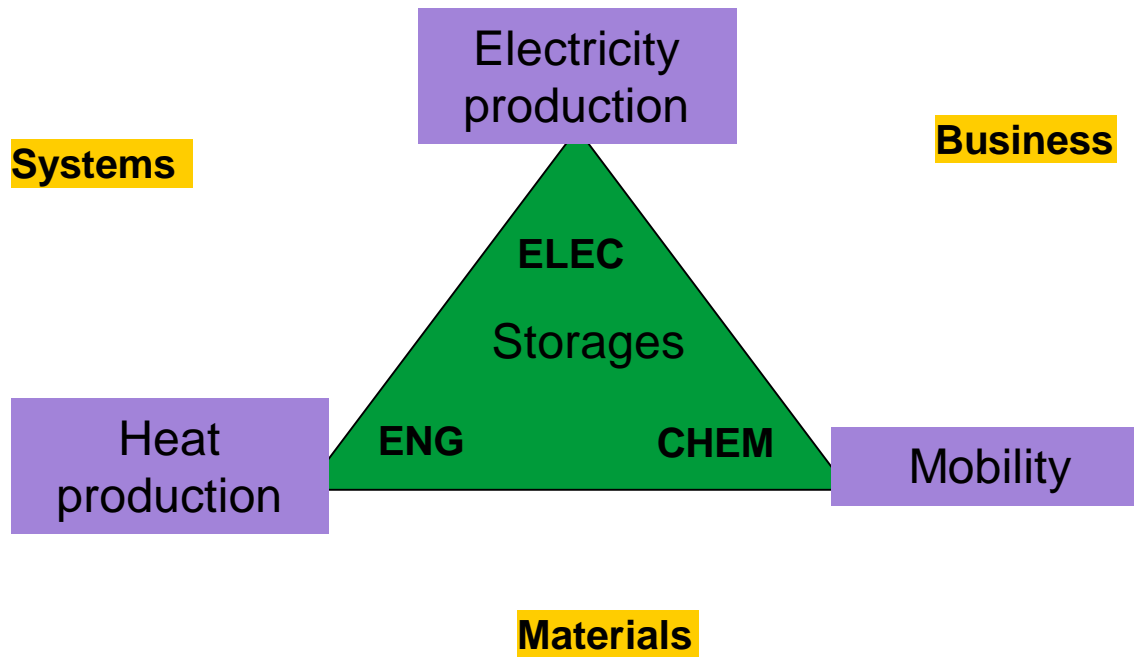
<https://youtu.be/mK41f24IX1k>

Energy Transition

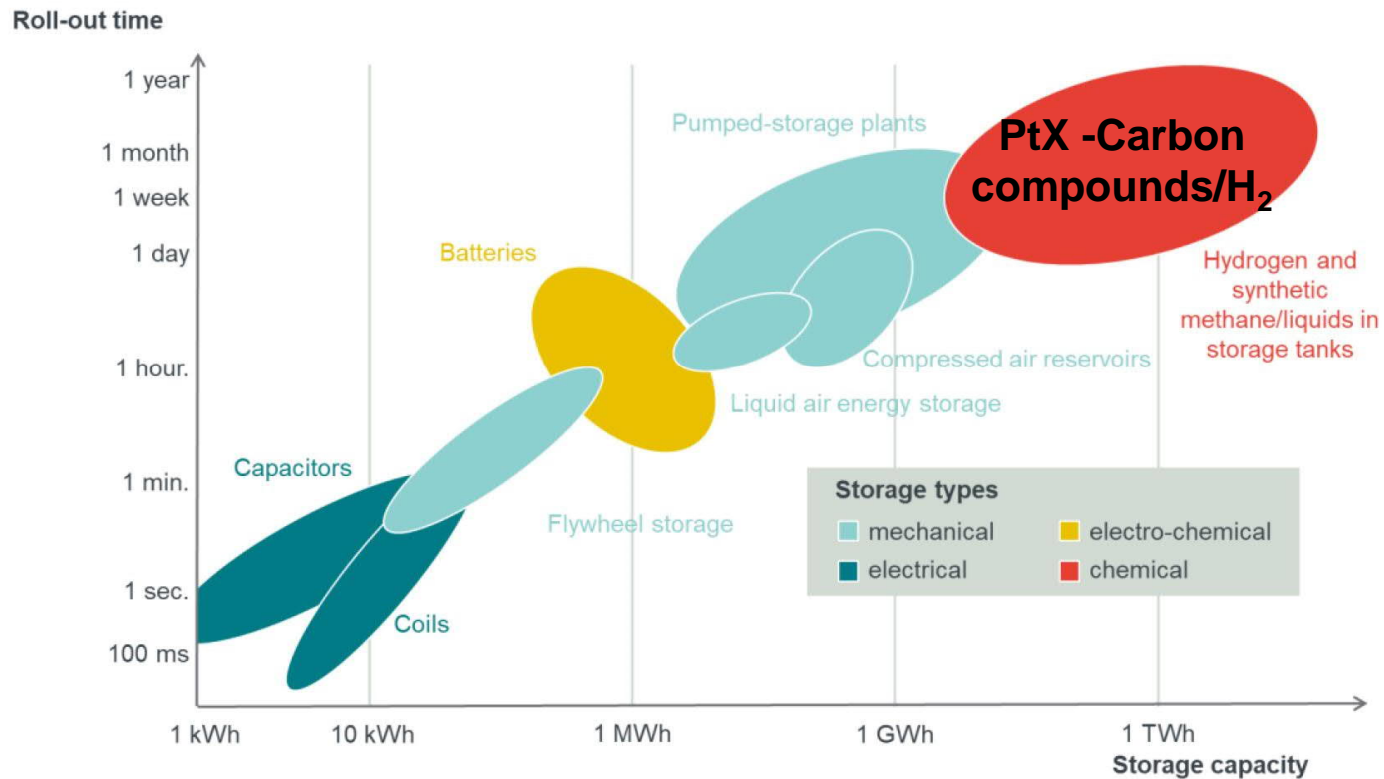


Institute of Energy of South East Europe

Energy Transition



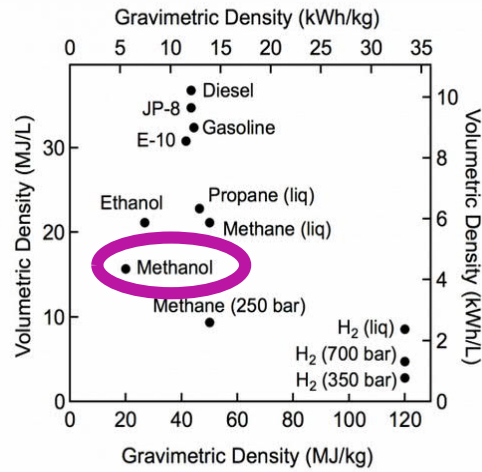
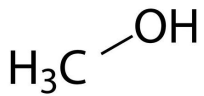
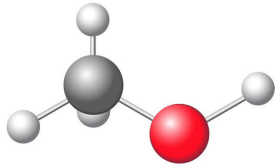
Where do we need power t X?



Methanol: a clean-burning multipurpose fuel



Methanol



Comparison of specific energy (energy per mass or gravimetric density) and energy density (energy per volume or volumetric density) for several fuels based on lower heating values.

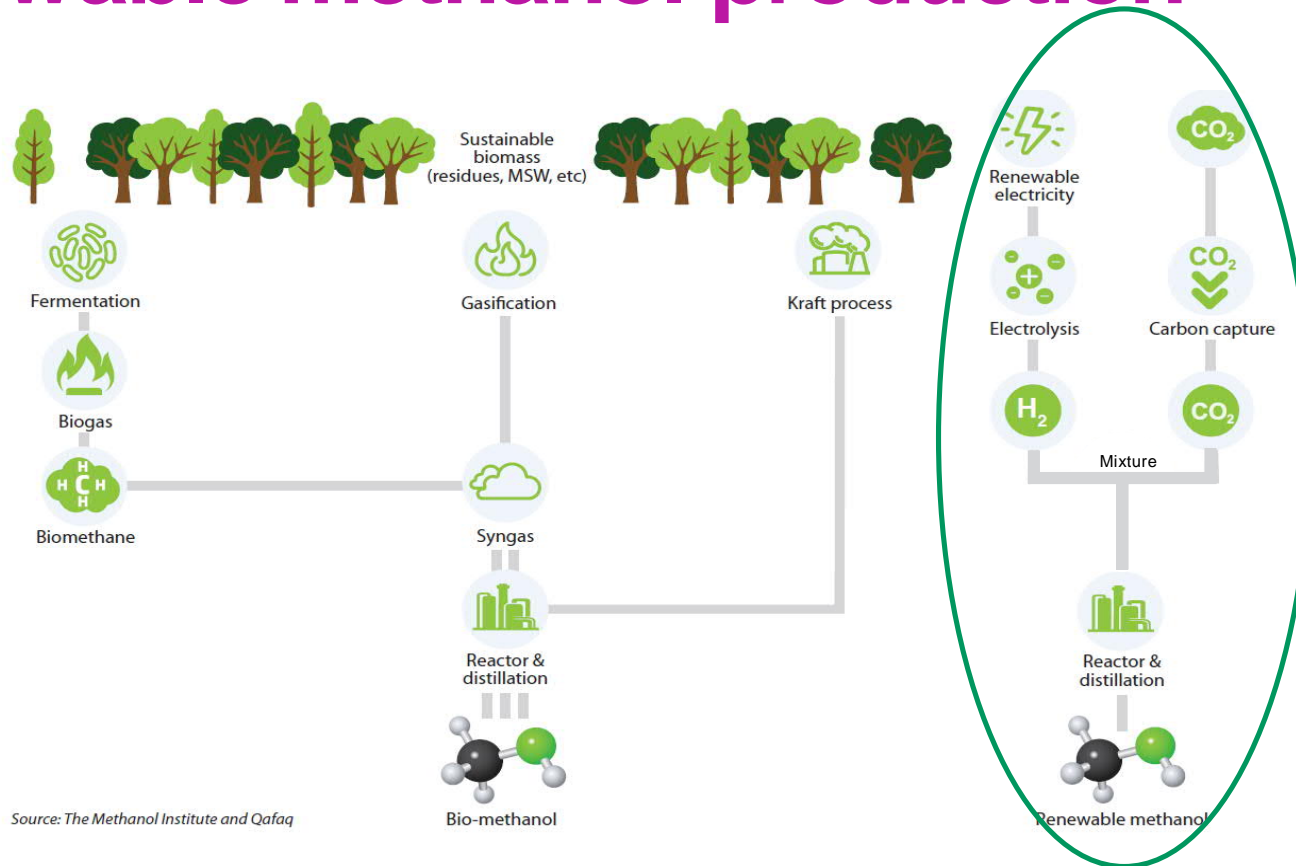


Emission reductions when compared to heavy fuel oil



Sources: Methanex, Investor Presentation, March 2019
ATA Markets Intelligence S.L., Renewable Methanol Report, December 2018
27.10.2021

Renewable methanol production



Source: The Methanol Institute and Qafaq

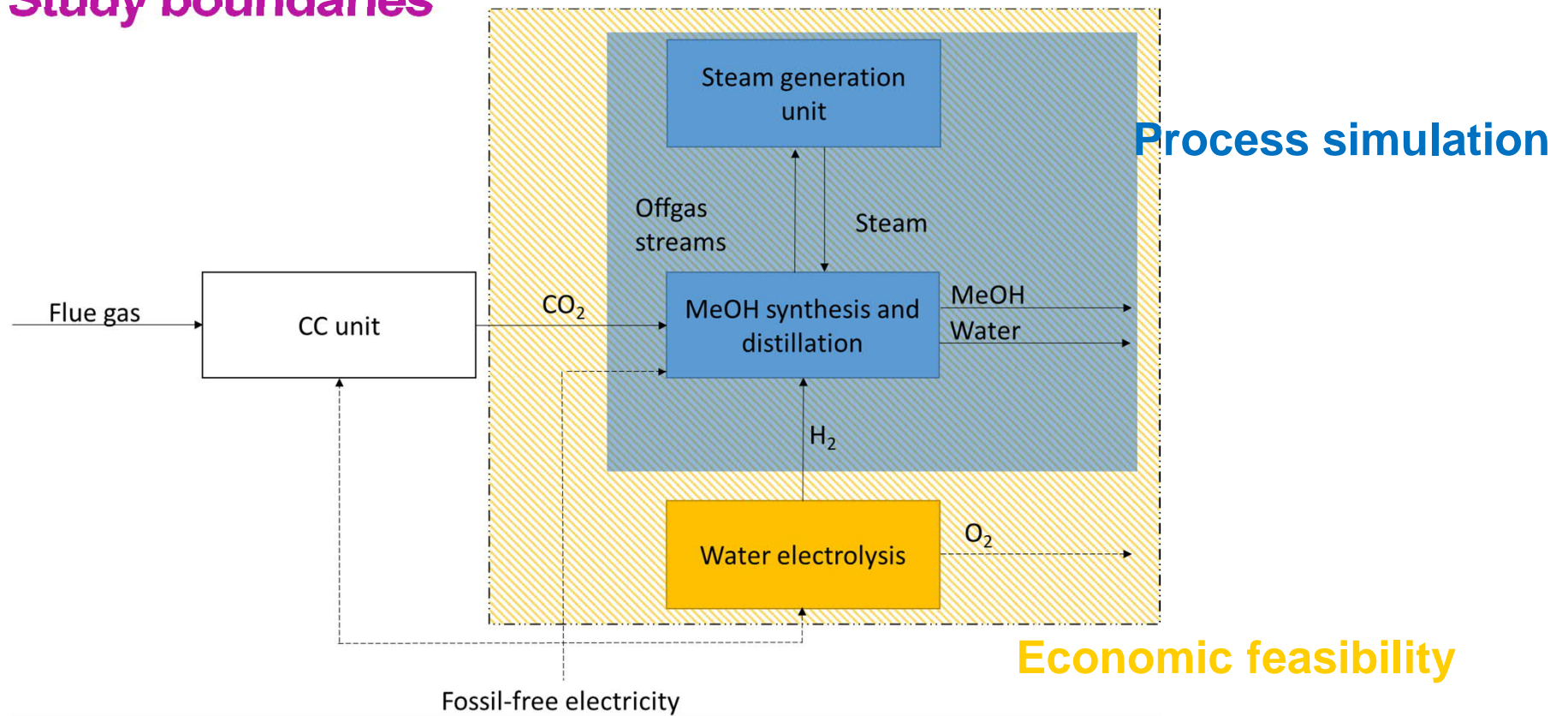
Source: ATA Markets Intelligence S.L., Renewable Methanol Report, December

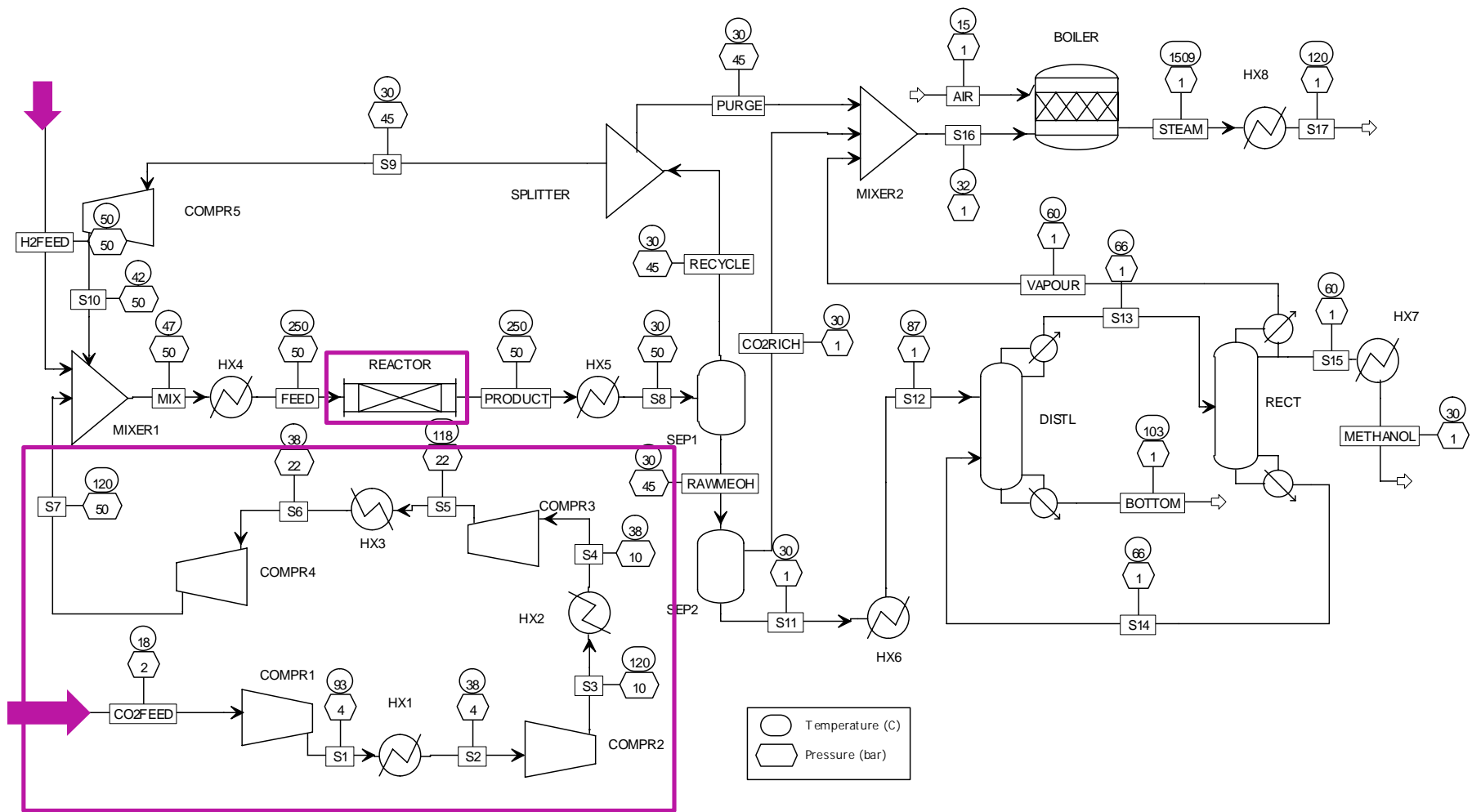
2018

Full system modelling Aspen Plus

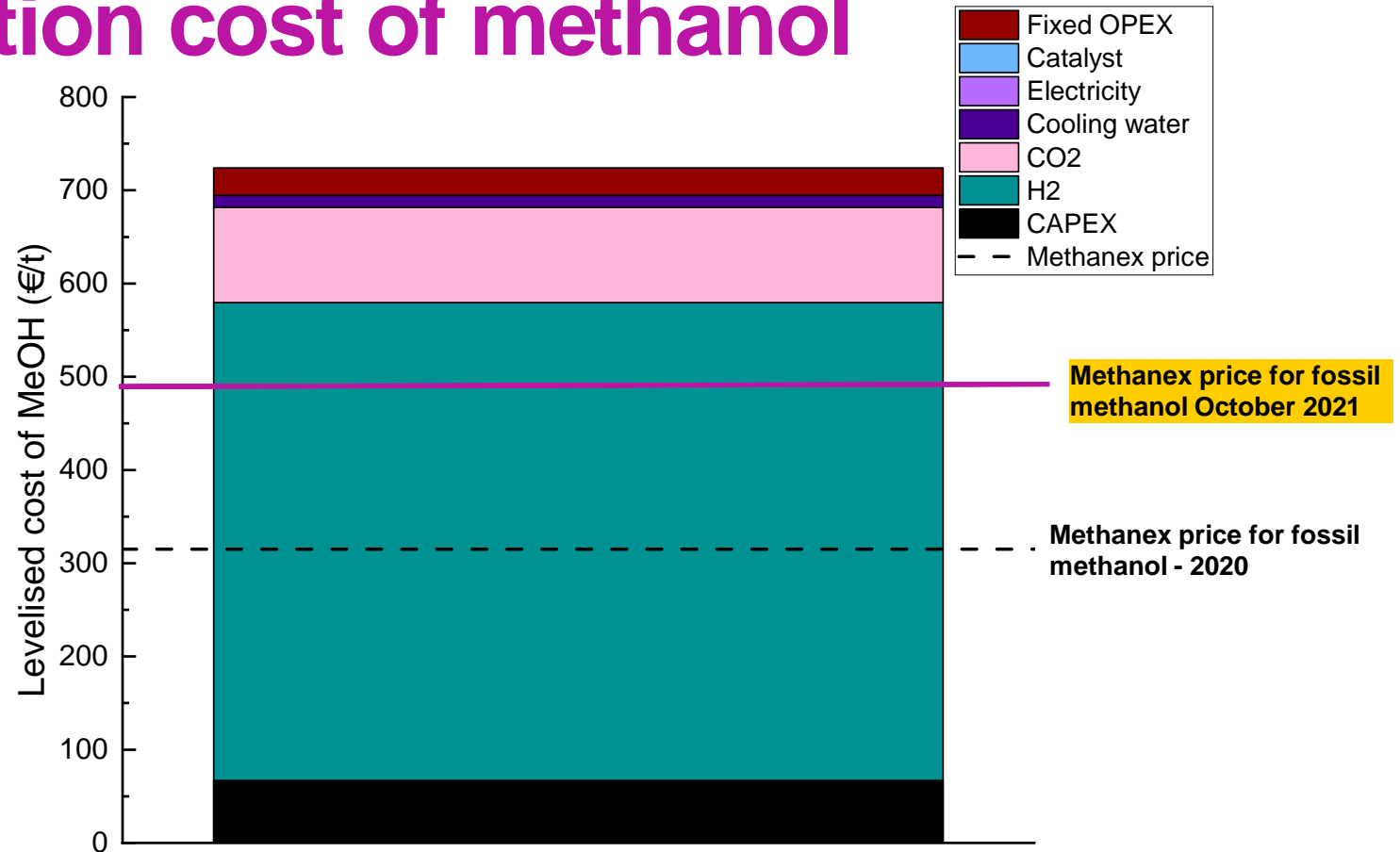
Methanol plant

Study boundaries

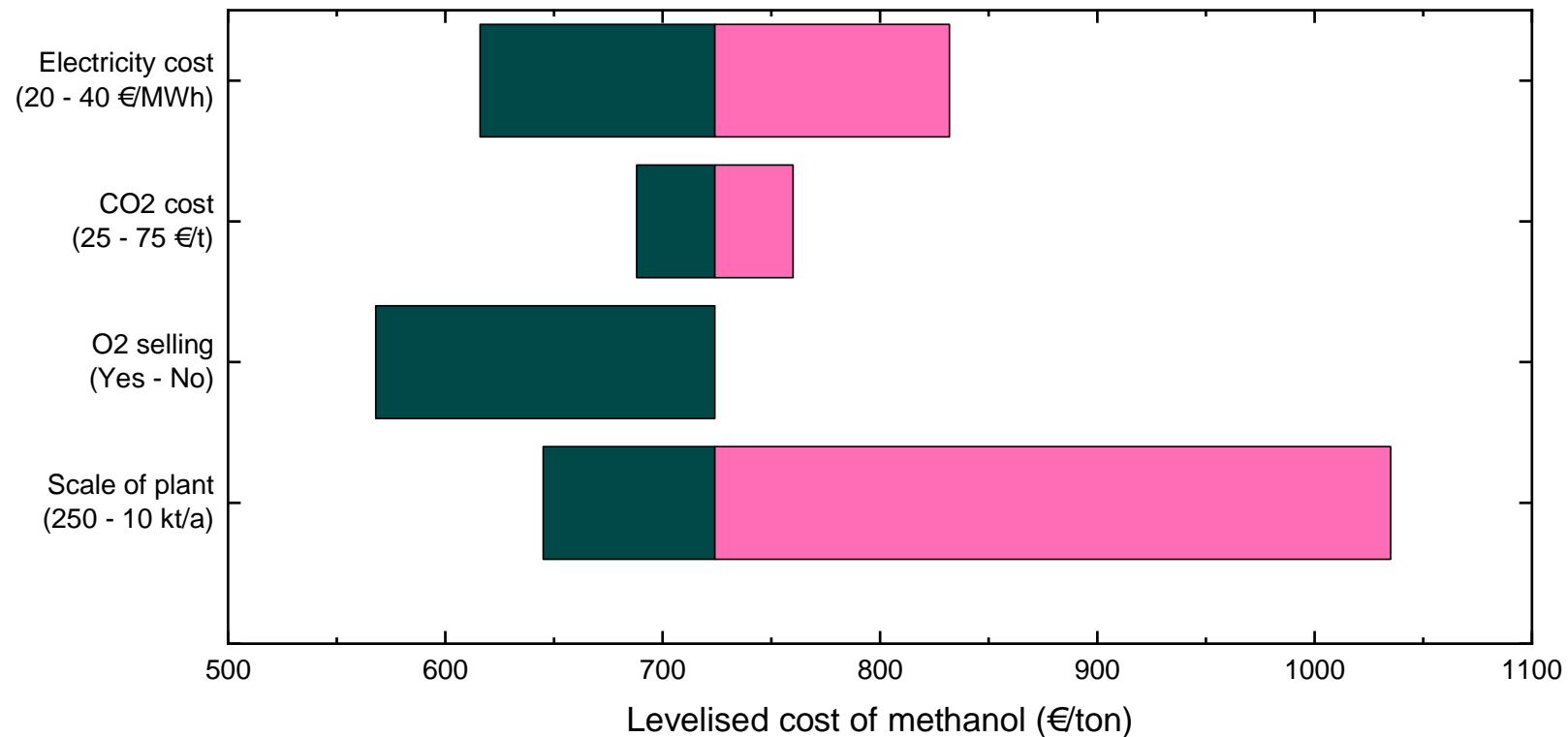




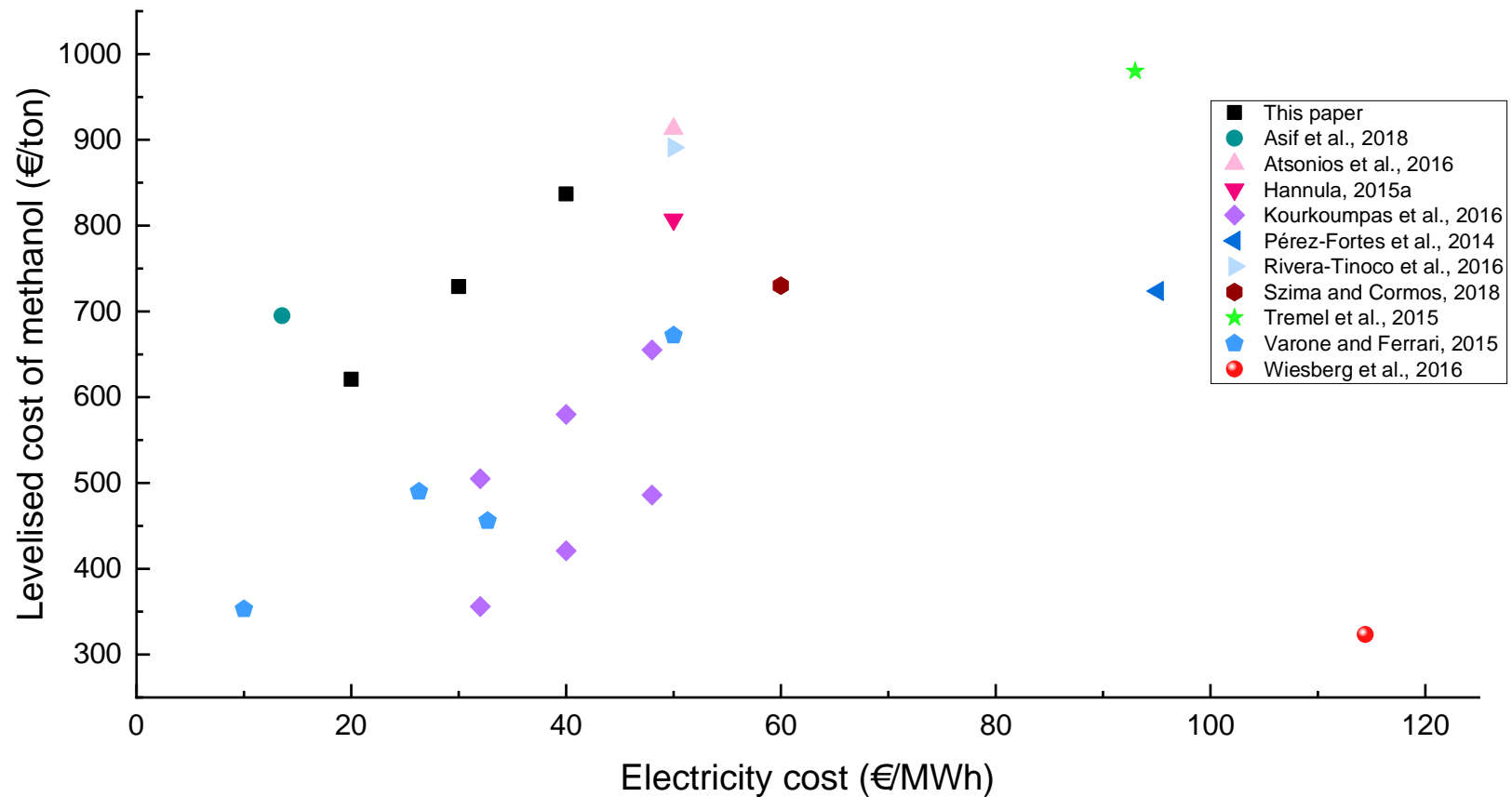
Production cost of methanol



Bottlenecks of economic viability



Comparison to other LCOMeOH studies



Reactor modelling

Computational Fluid Dynamics (CFD)

Computational Fluid Dynamics

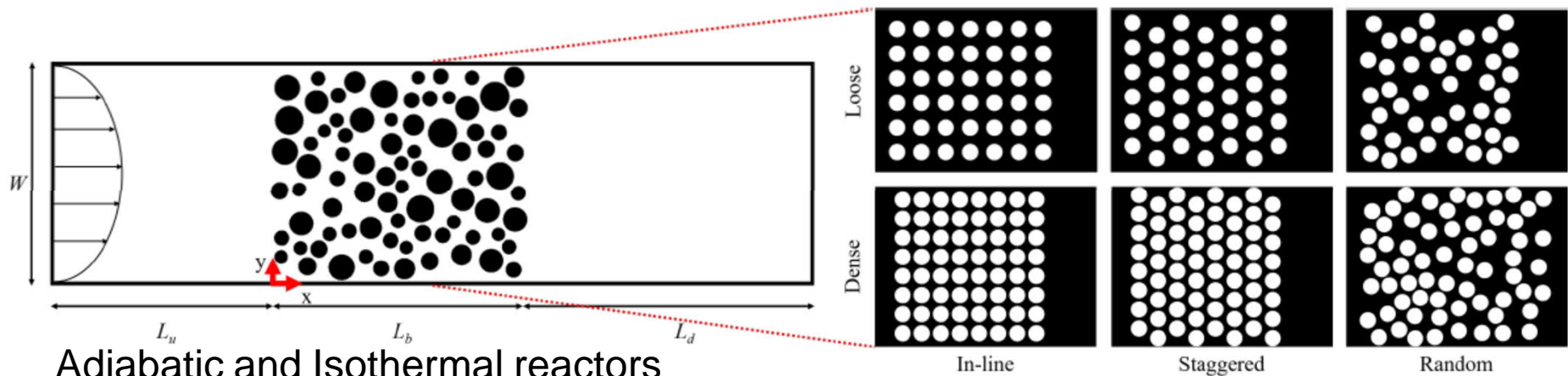
CFD modelling of multi-tubular and milli-scale reactors.



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Aim and objectives

Development of intensified cost-effective methanol synthesis process starting from H_2 and CO_2 using modular milli-scale reactor design.



Adiabatic and Isothermal reactors

Software:

OpenFOAM

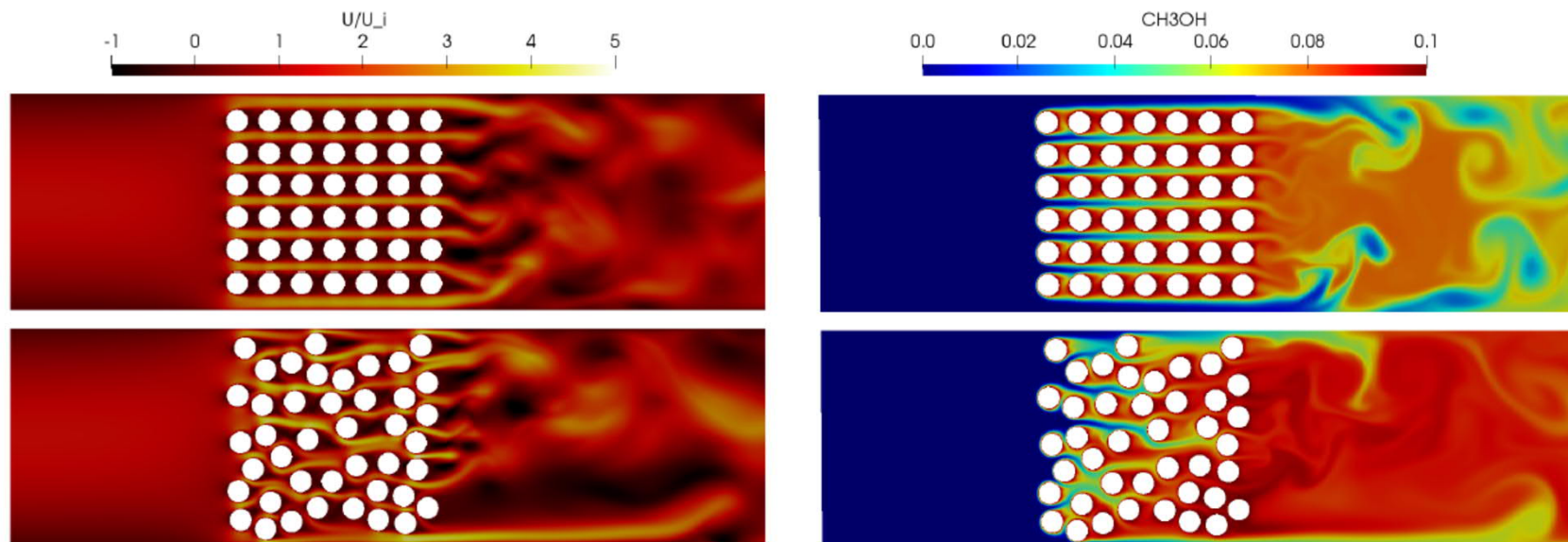
Izbassarov *et al* (2021)

<https://doi.org/10.1016/j.ijhydene.2021.02.031>

2D Fixed-bed Reactor



P2X
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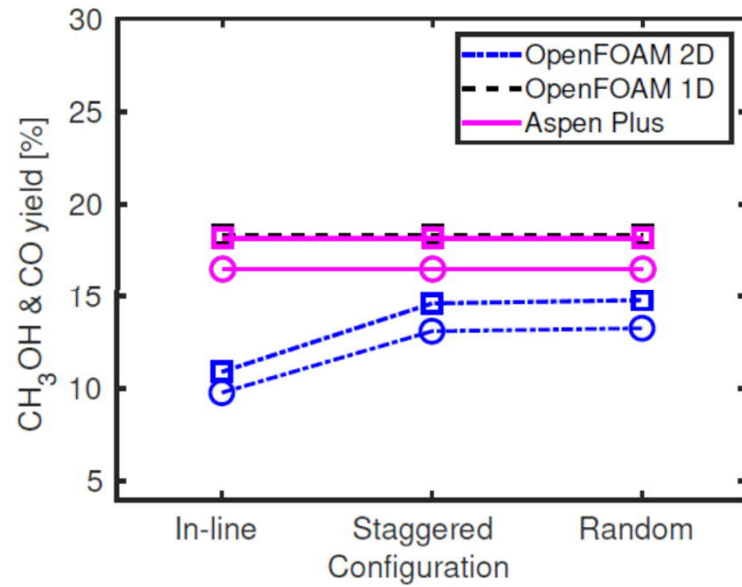


Adiabatic reactor

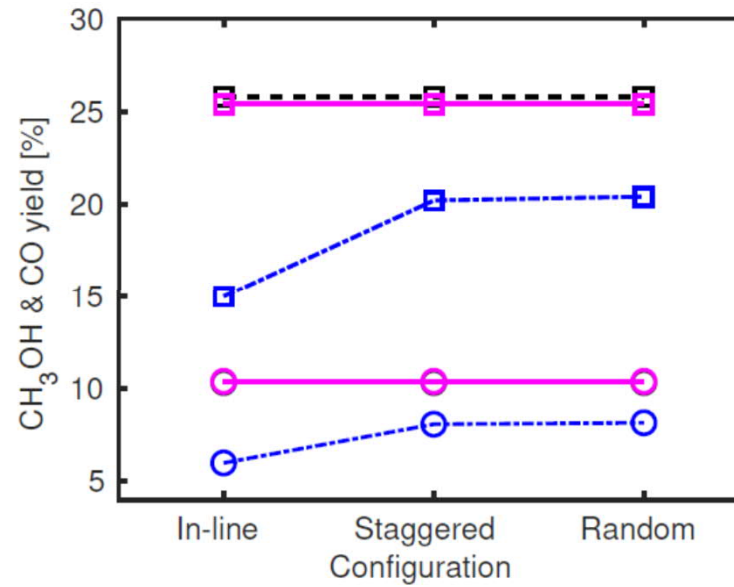
$$T_i = 523K, p_i = 5MPa, Re = 100, SV = 6 m^3/kg_{cat} h$$

2D Fixed-bed Reactor

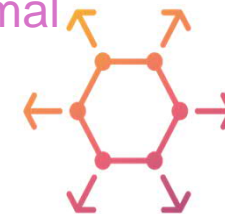
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Adiabatic



Isothermal



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Izbassarov *et al* (2021)

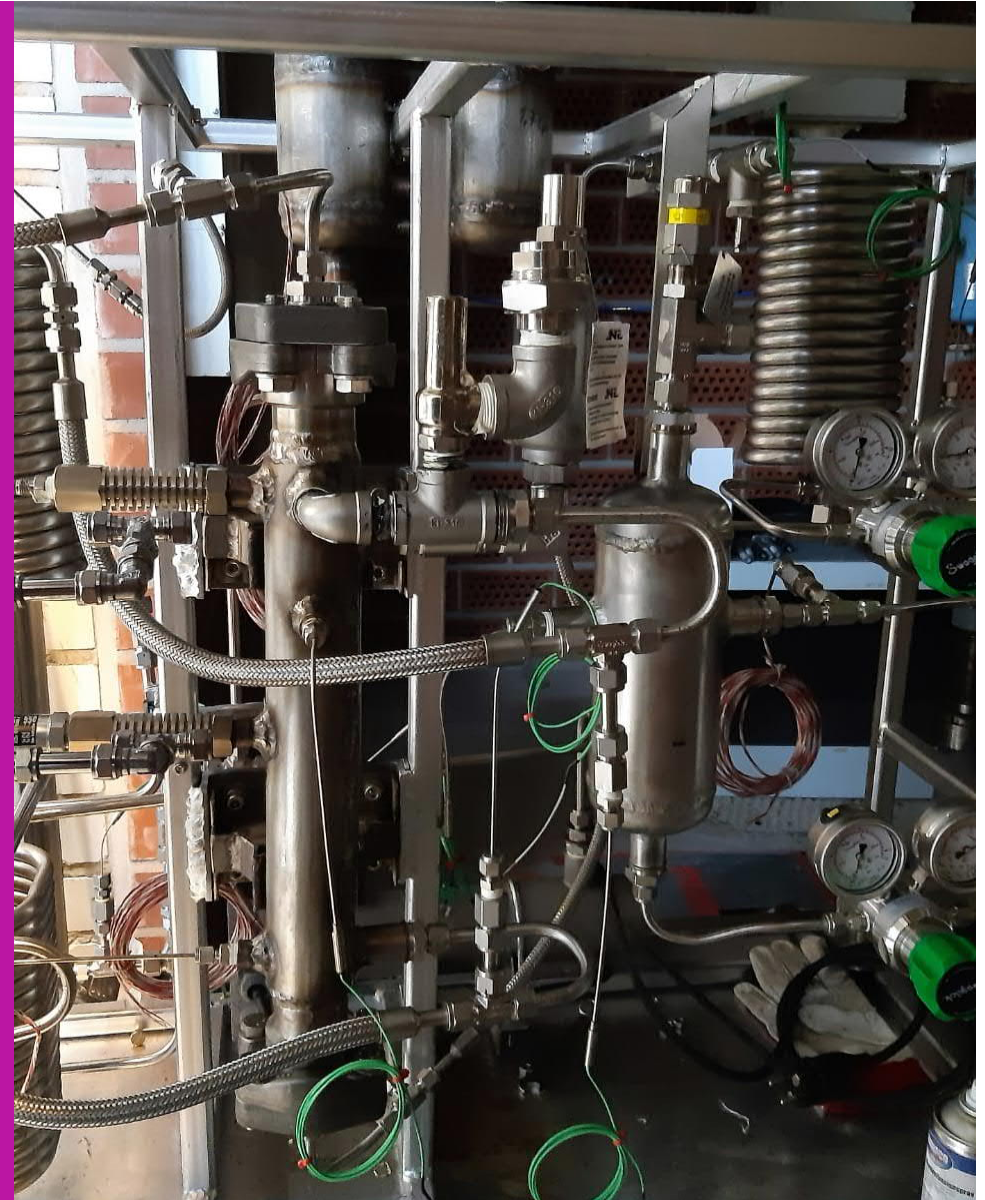
<https://doi.org/10.1016/j.ijhydene.2021.02.031>

Experimental studies

Lab-scale methanol synthesis reactor



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Experimental reactor system

Methanol synthesis from CO_2 and H_2

Process conditions

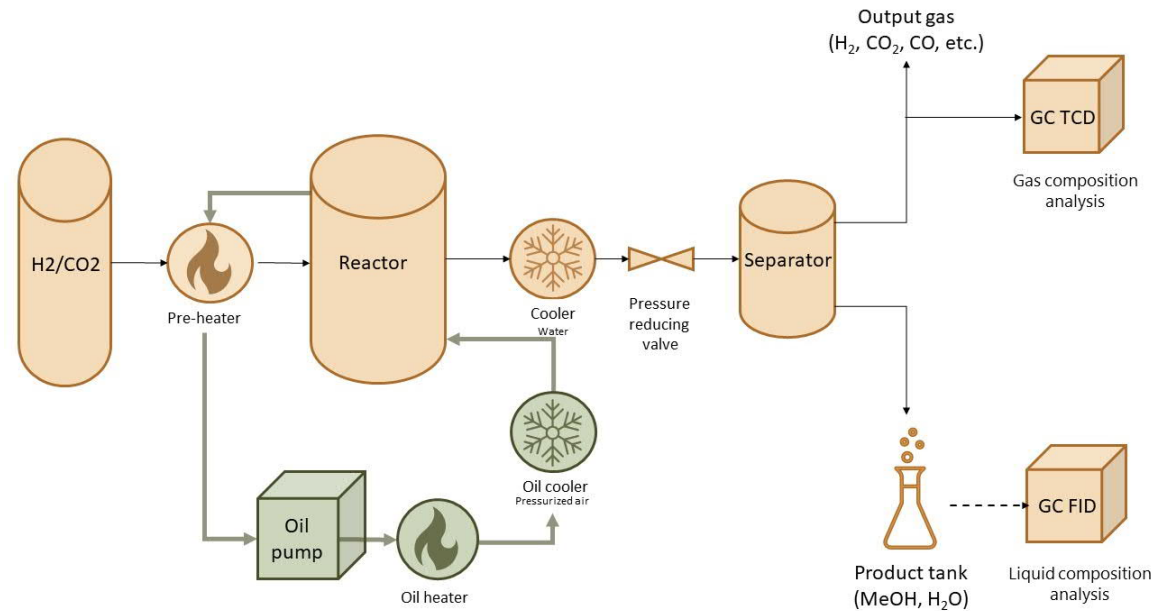
T: 200 – 250 °C

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