Attività di ricerca sui combustibili sintetici da idrogeno: modellazione e Life Cycle Assessment

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Mobilità Sostenibile: Bio-combustibili e infrastrutture, 11 dicembre 2019 - Napoli

Energy Systems and Turbomachinery Research Group

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- Thesists (Bachelor and Master)
  - Around 25 students per year
  - Energy, Mechanical, Vehicles Engineering

International and national collaborations

University of Zaragoza (Spain)

University of Duisburg-Essen (Germany)

Warsaw University of Technology (Poland)

University of Cassino and Southern Lazio (Italy)

Research activities on electrofuels: Intro, assumptions and research objectives

<u>Electrofuels/Synthetic fuel</u>: emerging class of potential more sustainable fuels that are made by storing <u>electrical energy</u> from <u>renewable sources</u> in the chemical bonds of liquid or gas fuels.

- ❑ Long term storage
- ❑ Lowering emissions

→

<u>RESEARCH GAP</u>:

- ❑ Efficiency of the overall pathway (electricity-end use)
- ❑ Associated emissions/impact- Lower than the actual?

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PROCESS MODELING

SYSTEM INTEGRATION

PROCESS OPTIMIZATION

LIFE CYCLE ASSESSMENT

Research activities on electrofuels: Intro, assumptions and research objectives

Modelling and simulation of electrolfuel synthesis routes from H_2 and CO_2 and/or N_2

Comparison on the basis of efficiencies, specific consumption and CO_2 emissions for the same amount of feed hydrogen

Life Cycle Assessment of the considered (Cradle-to-Gate) for different functional units, energy mix and CO_2 sources

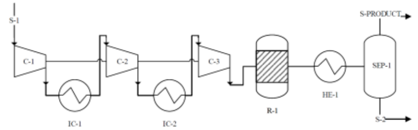
Investigated fuels and conversion pathways

Electricity (RES)

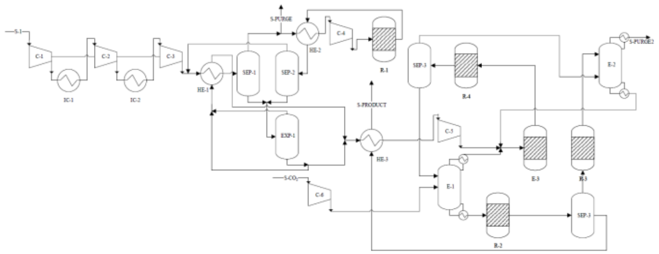
PEM electrolyzer

H_2

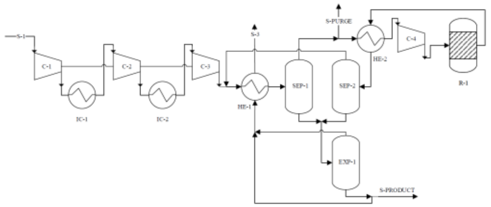
CO_2 → Sabatier Process → Methane



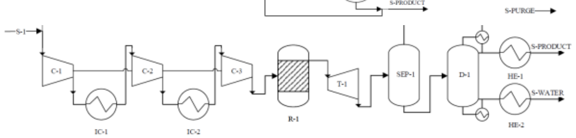
CO_2, N_2 → Bosch-Meiser Process → Urea



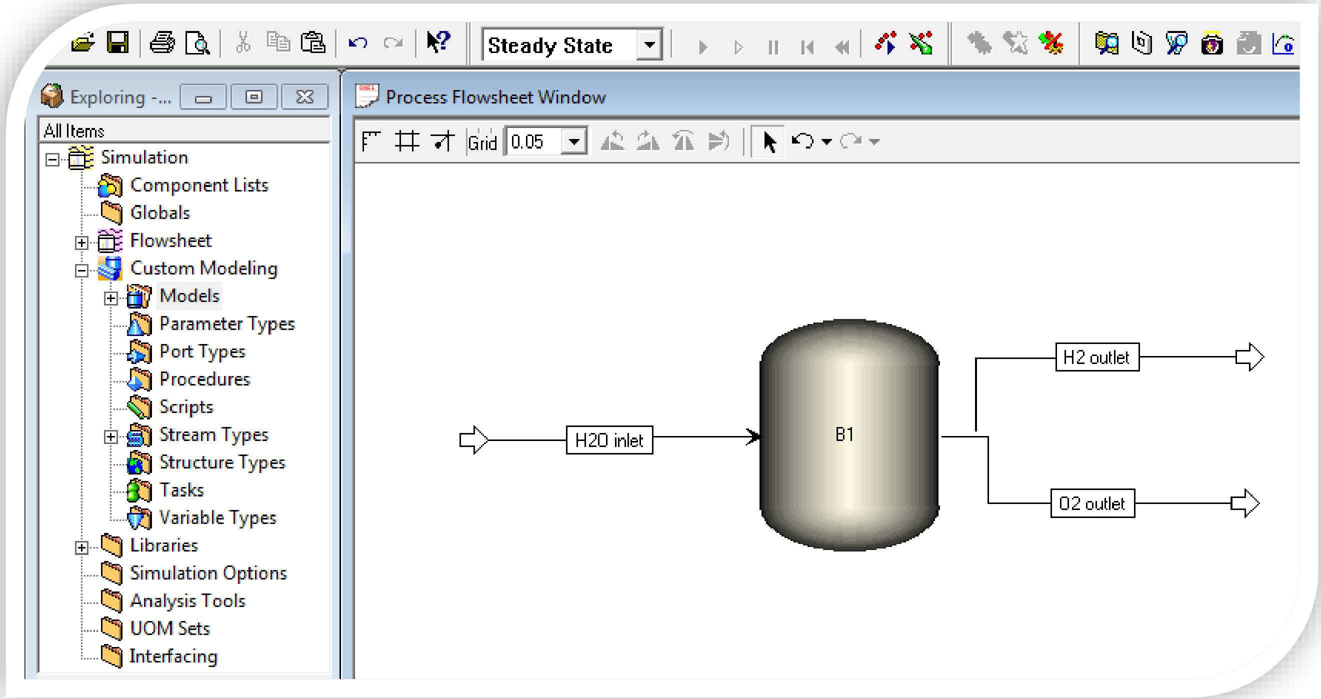
N_2 → Haber-Bosch Process → Ammonia



CO_2 → CO_2 hydrogenation → Methanol



Electrolyzer model



McPhy
Driving clean energy forward

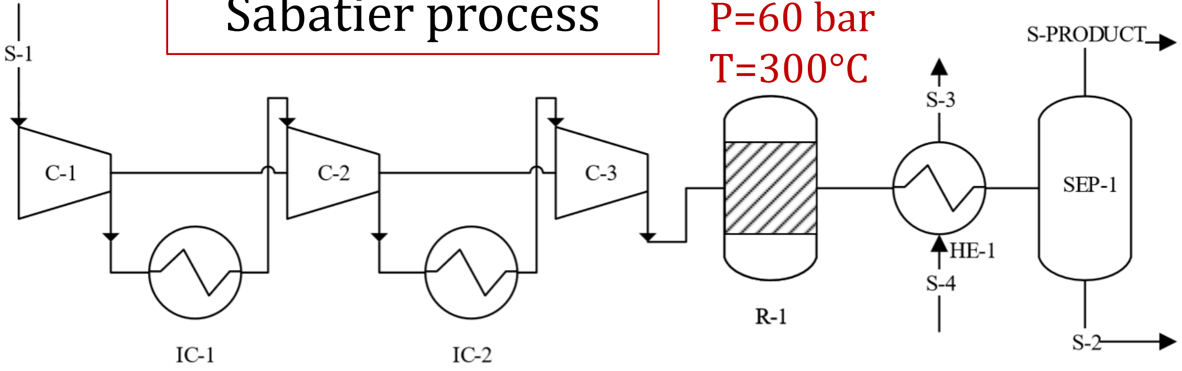
aspentech

- Modelling of alcaline and PEM electrolyzer in Aspen Custom Modeler and Aspen Hysys
- Experimental validation with a 30 kW alcaline electrolyzer and a mini PEM electrolyzer (ongoing)

H_2 conversion pathways models

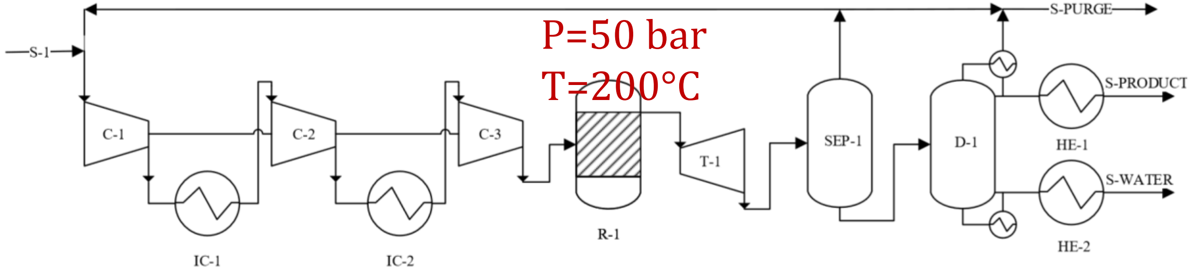
Methane
Sabatier process

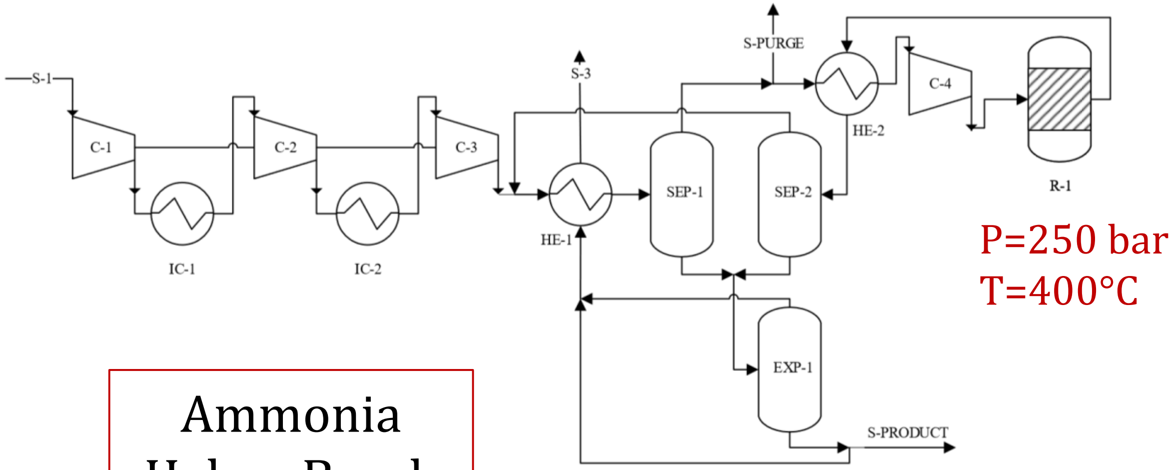
P=60 bar
T=300°C



Methanol
CO2 dehydrogenation

P=50 bar
T=200°C

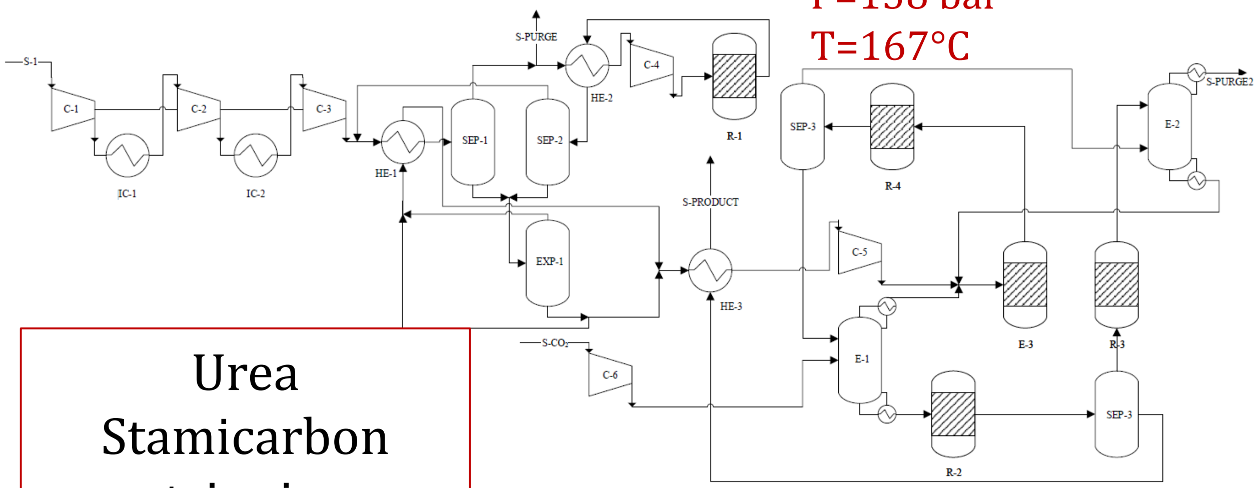




P=250 bar
T=400°C

Ammonia
Haber-Bosch

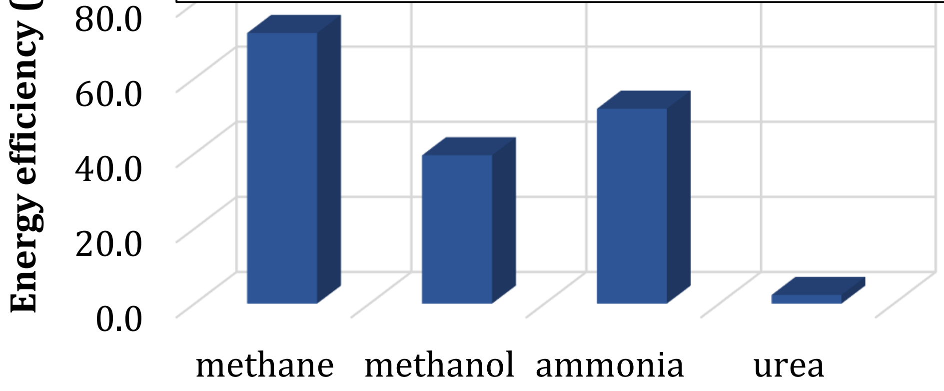
P=138 bar
T=167°C

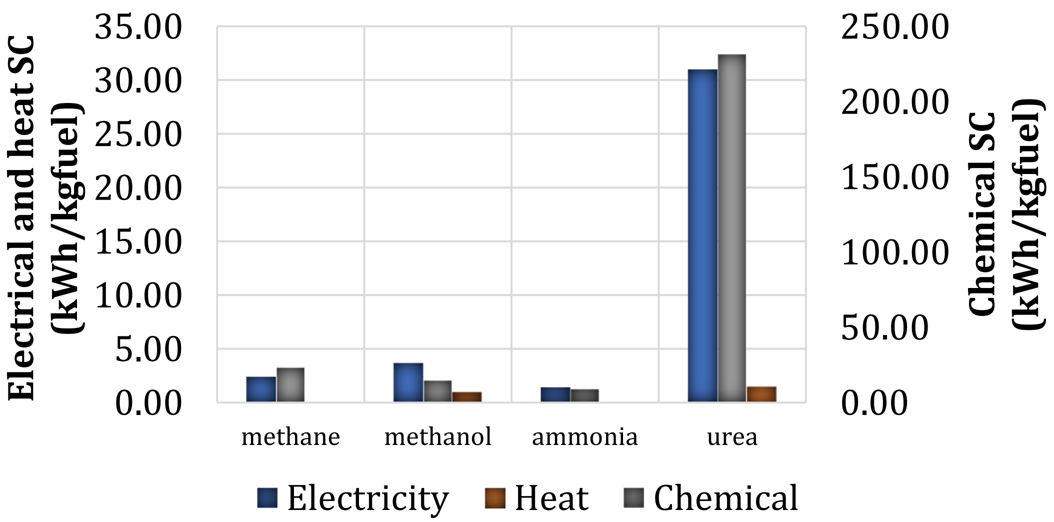


Urea
Stamicarbon
stripping

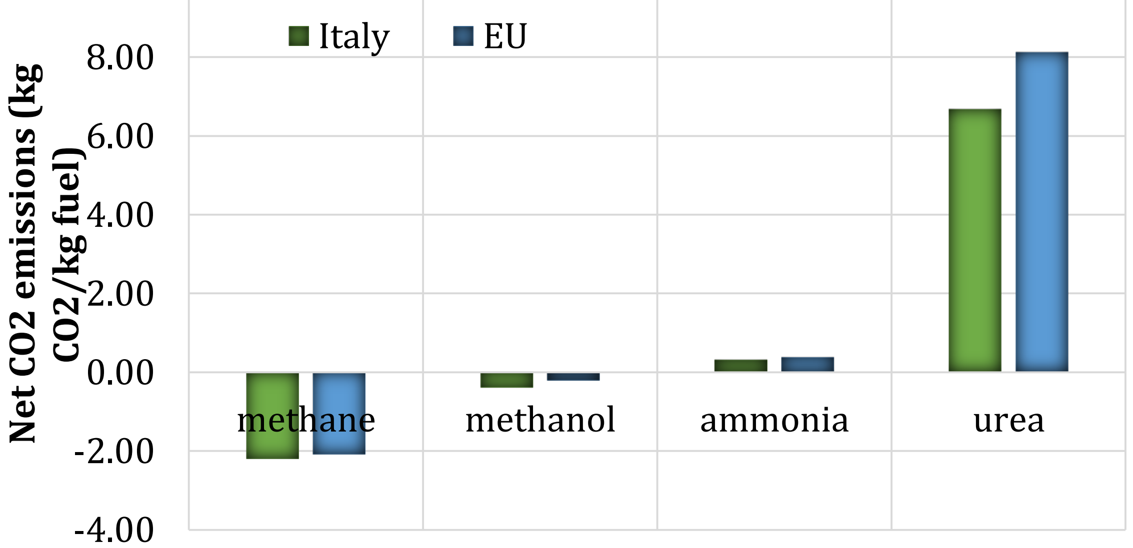
H_2 conversion pathways models – Results 1

$$\eta_I = \frac{\dot{m}_{fuel} LHV_{fuel}}{\sum_{i=1}^{n} \dot{m}_{syn,in,i} LHV_{syn,i} + \sum_{j=1}^{m} Q_{in,j} + \sum_{k=1}^{q} W_{in,k}}$$





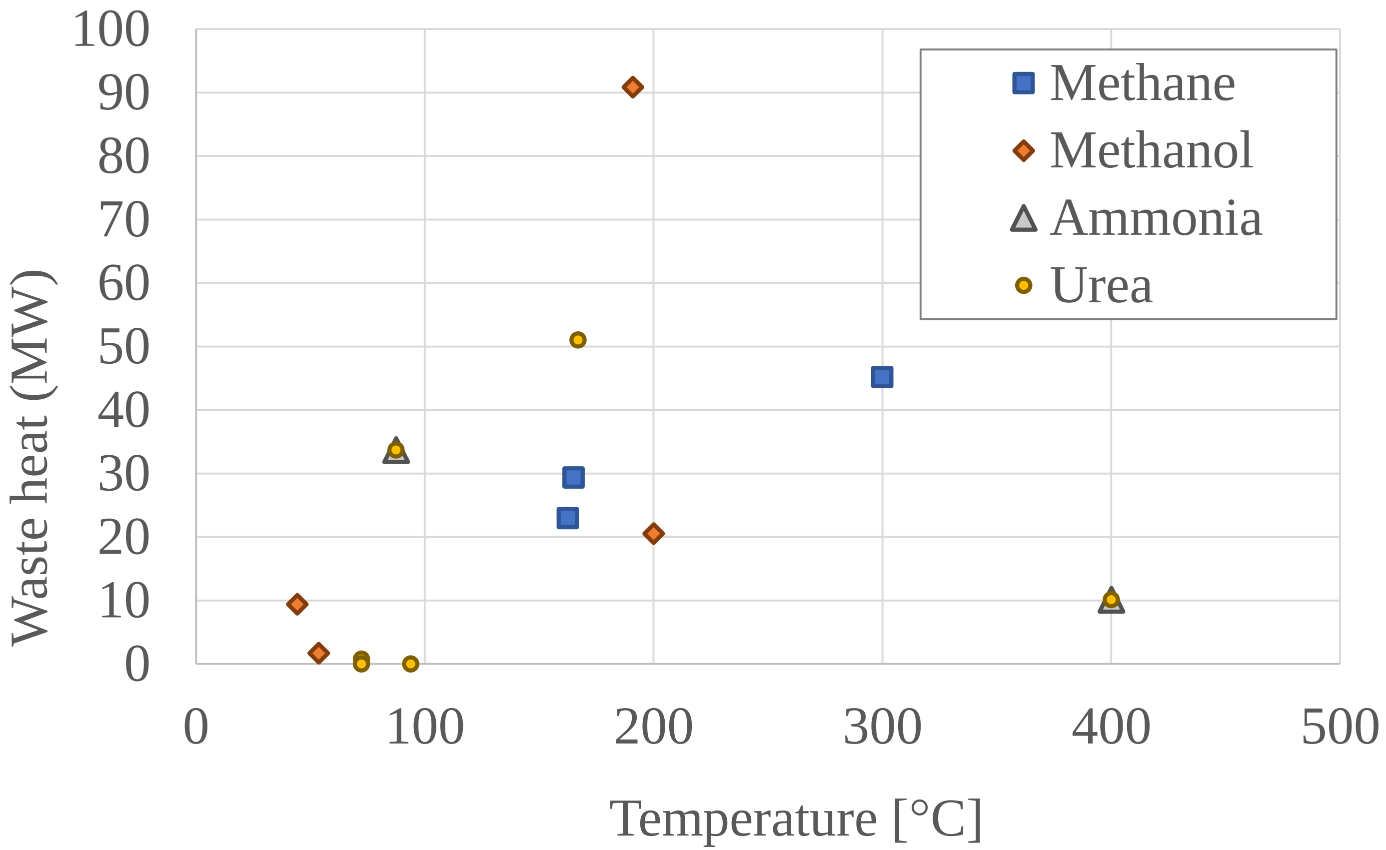
$$CO_{2,net} = CO_{2prod,out} - CO_{2feed,in} + CO_{2,eq.heat} + CO_{2eq.el}$$



Energy efficiencies up to 70% (disregarding the electrolyzer)

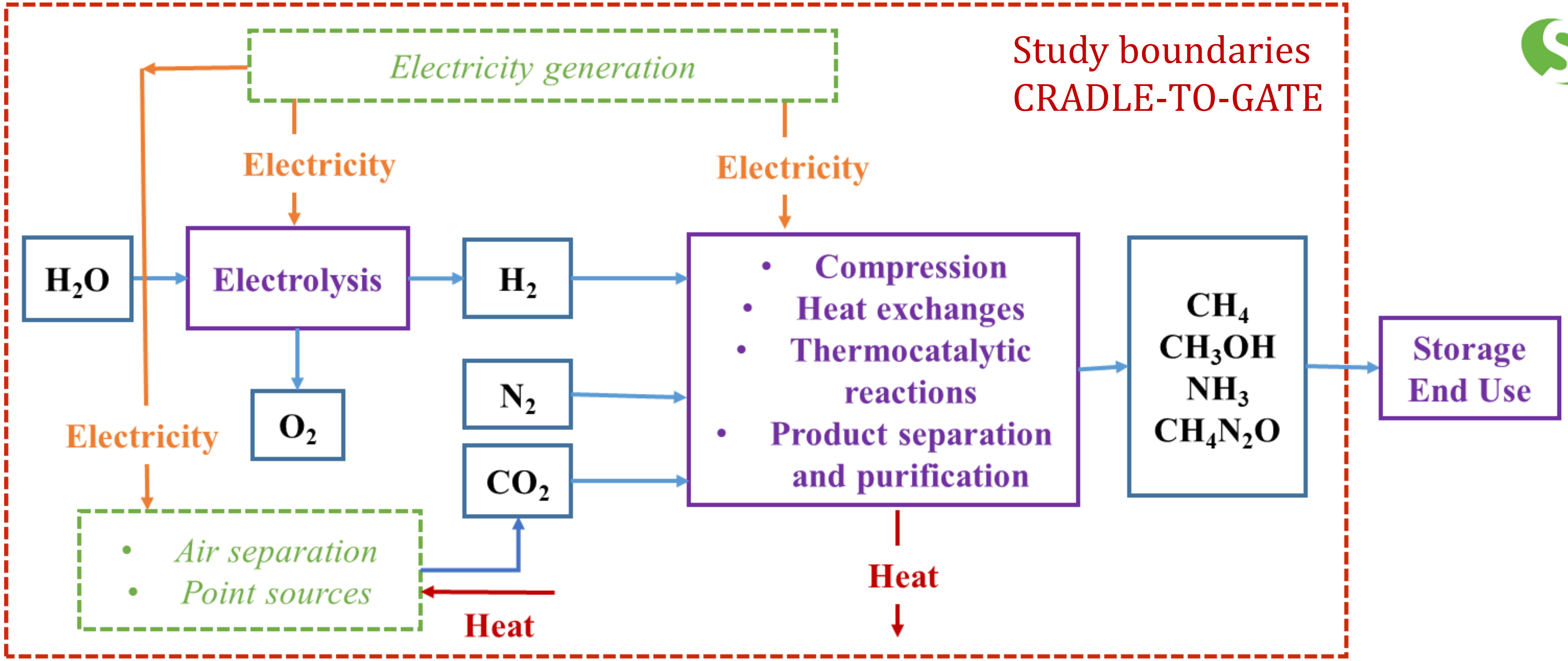
CO_2 net emissions highly dependent on CO_2 emission intensity (kg_{CO2}/kWh) for electricity and heat production

H_2 conversion pathways models – Results 2



Power-to-Fuel plants release a significant amount of heat,most of which could be fruitfully employed

Life Cycle Assessment – Study boundaries



Assumptions:
- No waste scenario
- No plant commissioning and decommissioning (impact<5%)

Life Cycle Assessment – Analyses

SimaPro

Impact assessment for different functional units

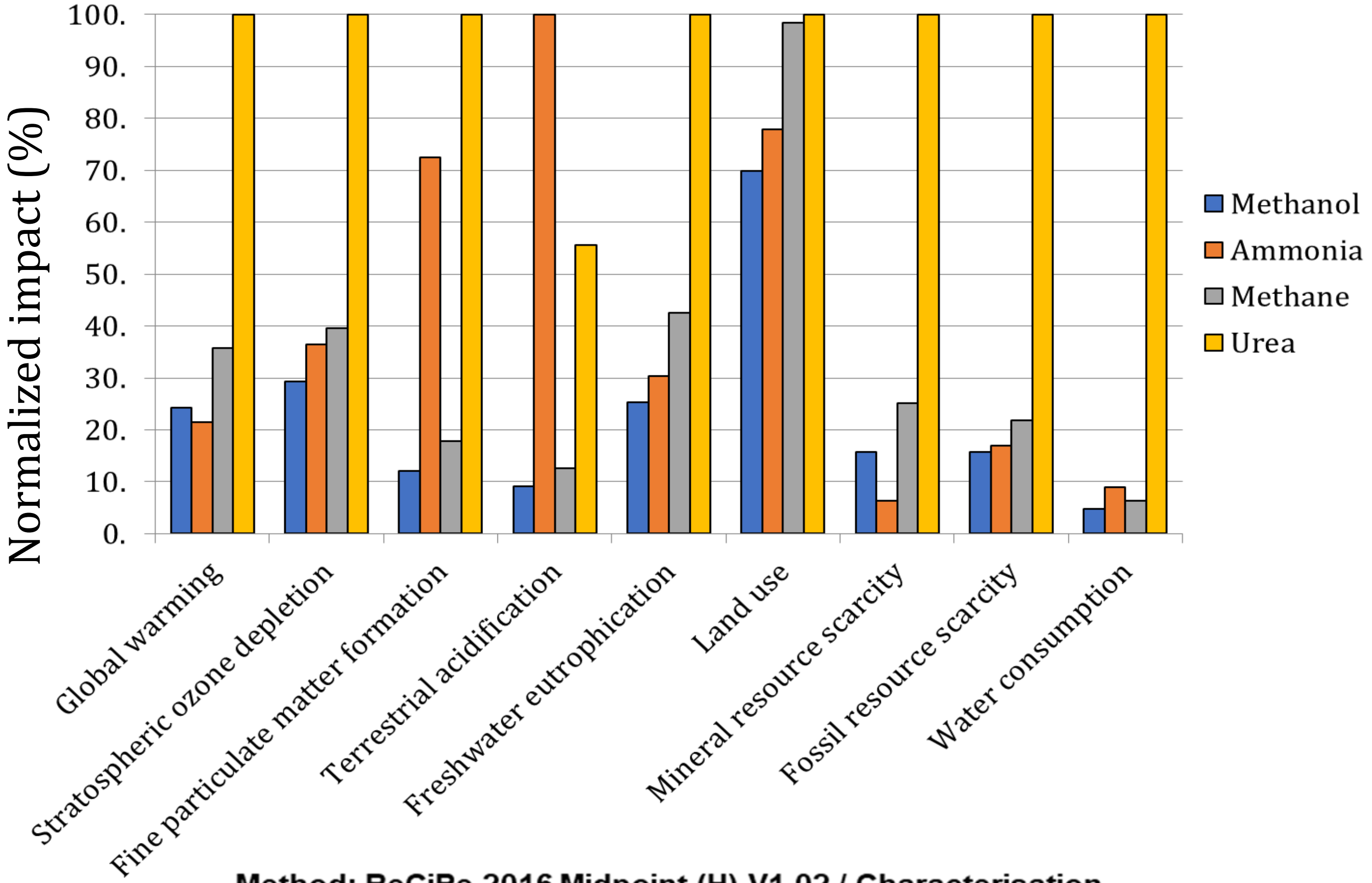
- 1 kmol H_2 in
- 1 GJ energy out

Process contribution analysis

Sensitivity analysis

- Energy mix
- CO_2 source

Life Cycle Assessment – Impact assessment results



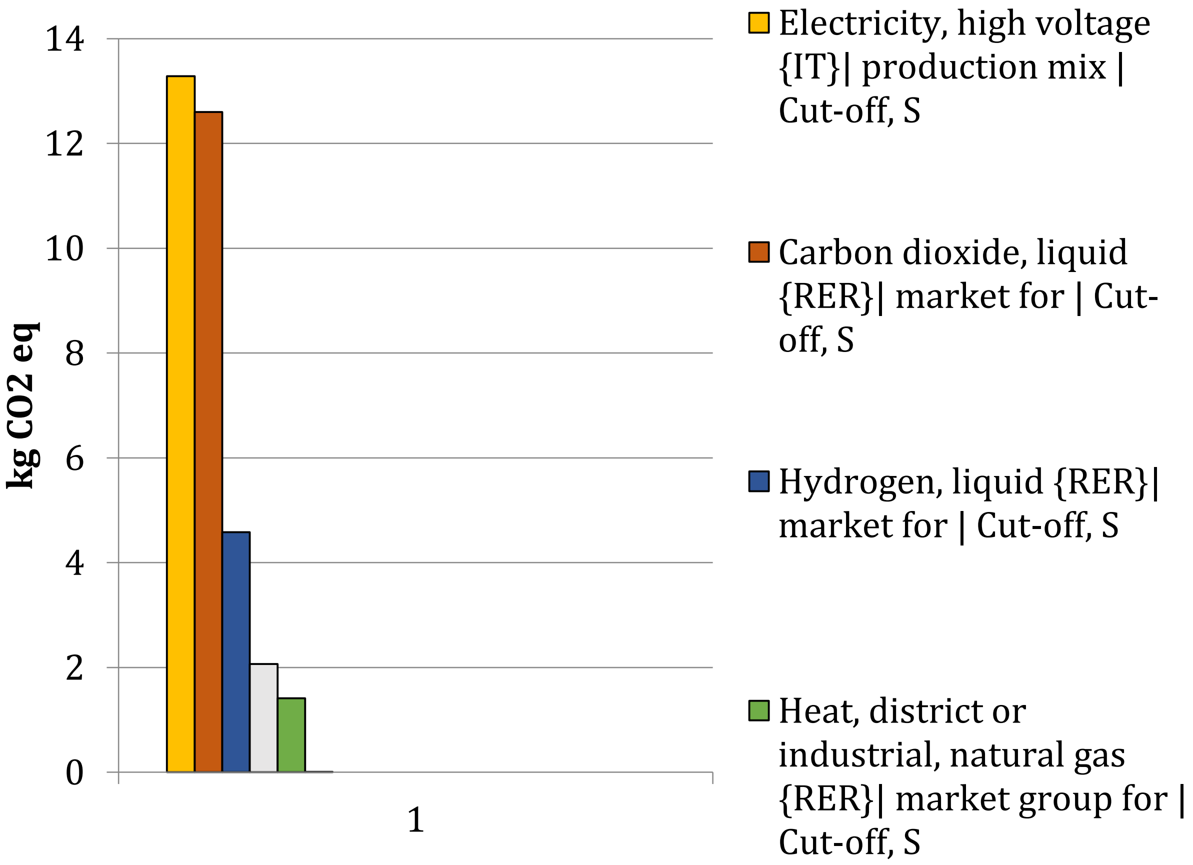
Method: ReCiPe 2016 Midpoint (H) V1.02 / Characterisation

- ❑ 1 kmol H2 feed for all the pathways
- ❑ Italian actual energy mix, CO_2 from DAC

<u>Results:</u>

- ❑ Methanol and ammonia result the pathways with the lowest impact on all the indicator
- ❑ Using a different energy mix or CO_2 source can drastically change the results

Life Cycle Assessment – Process contribution



- For all the pathways the considered indicators are mainly dependent on the electricity mix and the CO_2/N_2 source

→ Sensitivity analysis on energy mix and CO_2/N_2 source

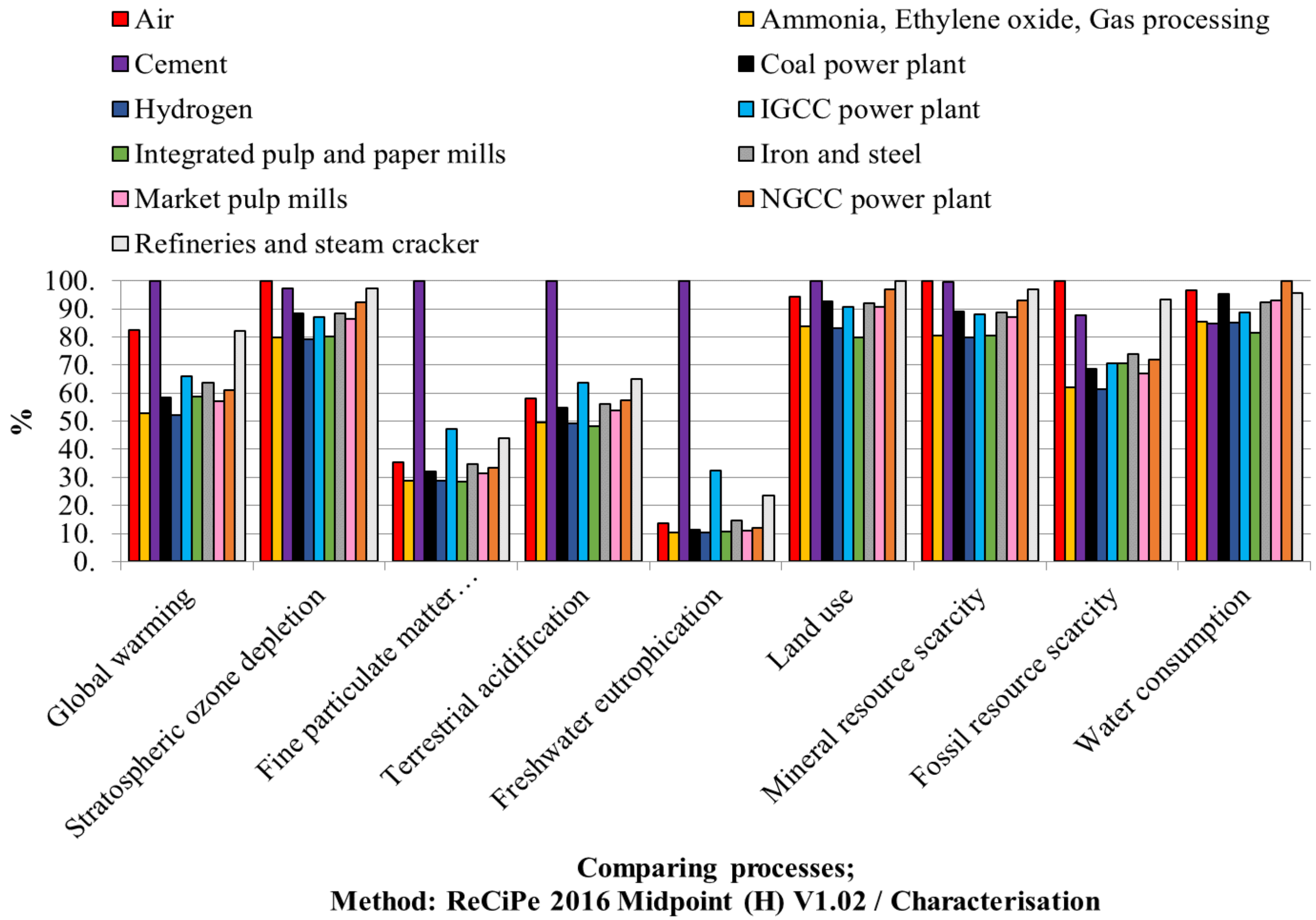
Life Cycle Assessment – CO_2 source sensitivity analysis

Different CO_2 point sources and DAC were investigated, using literature data.

type of CO_2 source	CO_2 concentration	average energy demand/(GJ (t $CO_{2,product}$)$^{-1}$)			
		electricity	heat	natural gas	coal
air	400 ppm	1.29		4.19	
NGCC power plant	3−4%	1.60			
refineries and steam cracker	3−13%	0.91	3.16		
coal power plant	12−15%	1.22			
integrated pulp and paper mills	7−20%	0.04		1.57	
market pulp mills	7−20%	1.03			
iron and steel	17−35%	0.87	0.95		
cement	14−33%	0.09			3.35
IGCC power plant	1/40%[b]	0.61			0.81
ammonia	≈100%	0.40	0.01		
ethylene oxide	≈100%	0.40	0.01		
gas processing	≈100%	0.40	0.01		
hydrogen	≈100%	0.35			

Assen N., Muller L. J., Steingrube A., Voll P. and Bardow A., Selecting CO2 Sources for CO2 Utilization by environmental-merit-order curves, Environmental Science and Technology, 2016, 50, 3, 1093-1101

Life Cycle Assessment – CO_2 source sentivity analysis results



Case study: SNG production with Italian 2030 energy mix

The most sustainable CO_2 sources are **hydrogen production plants** and **integrated pulp and paper mills**, while DAC and cement plants proved to be critical for their heavy use of natural gas and coal.

Concluding remarks

- Modeling and LCA of electrofuel synthesis

- Some processes are promising in terms of energy efficiency and carbon footprint
- Plant optimization and the exploitation of the waste heat are crucial aspects for these technologies sustainability and profitability
- It is essential not to limit the analysis to the plant itself but a comprehensive LCA for several impact categories and broad system boundaries

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Future work

- CO_2 capture technologies modelling and integration in the plant
- Comprehensive LCA and avoided emission calculation

- End use scenarios

Grazie per l'attenzione!

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