Advancing CO_2 Capture: From Lab to Industry by Process Modelling

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Internal Seminar – Chemical Engineering Department

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Content of the presentation

- How I Got Involved in CO_2 Capture Research?
- Why studying CO_2 capture? Why do we need this?
- HECO2 – Saturn Project
- PhD Thesis
  - Experimental work
  - Modelling work
- Conclusion

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How I Got Involved in CO_2 Capture Research?

- 2017 (2020) – 2022: (Chemical) Engineering studies at ULiège
  - Master's thesis focused on industrial processes and modeling
    - 'Modeling of a CO_2 Purification Unit via a Liquefaction Process' (3B Fiberglass – ULiège)
- August 2022 – December 2022: Preparation of a FRIA grant proposal
  - 'Comparison Between Centralized and Decentralized Approaches for Methanol and Dimethyl Ether Synthesis from CO_2'
    - Grant rejected
- 2023 – Present: HECO2 Saturn Project – WP5: CO_2 capture on industrial processes
  - PhD linked to the project

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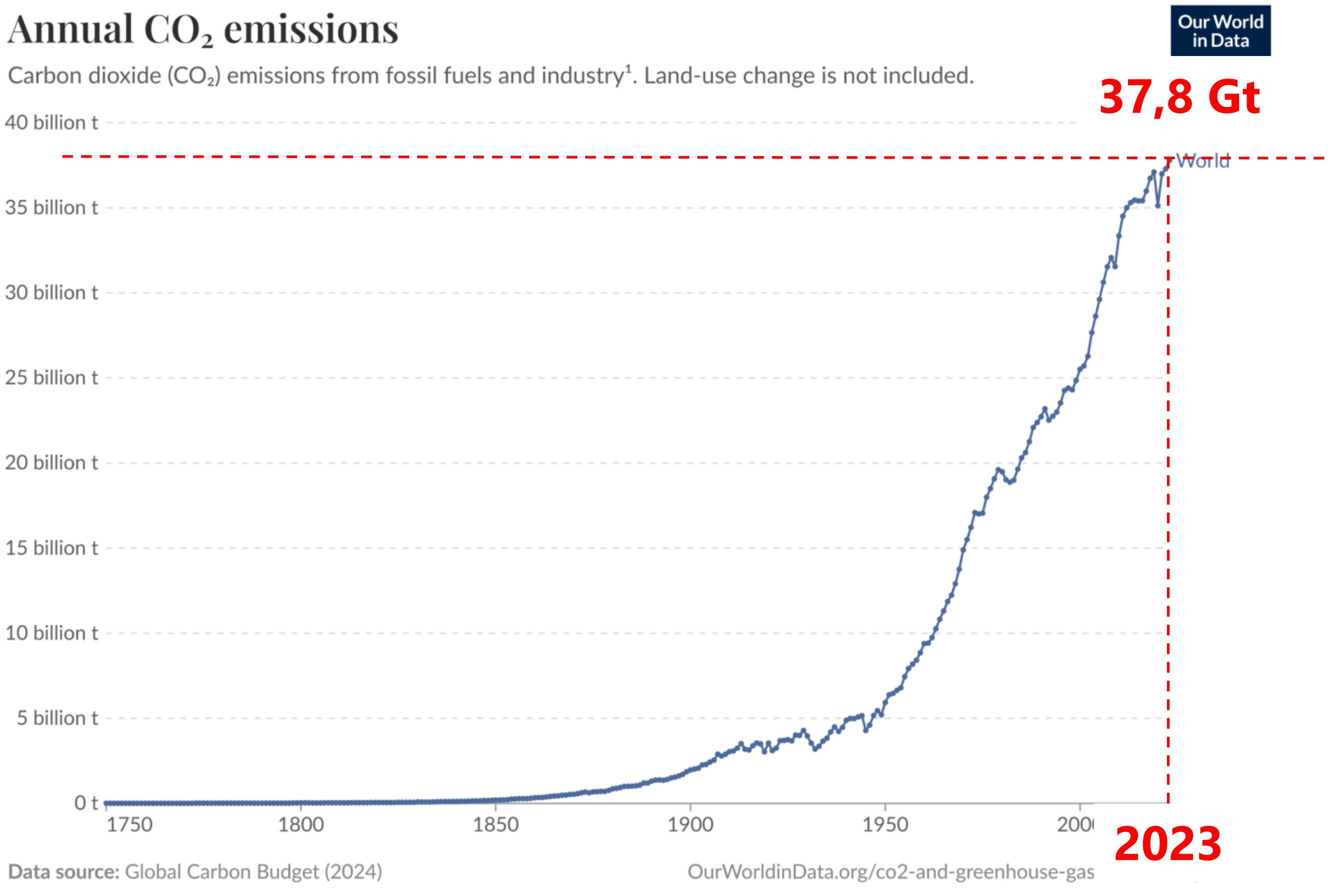
Why studying CO_2 capture?



Source : *https://ourworldindata.org/co2-emissions*

2023 : 83,4 Mt de CO_2

~2,2% of global emission

~20 kg/day/inh.

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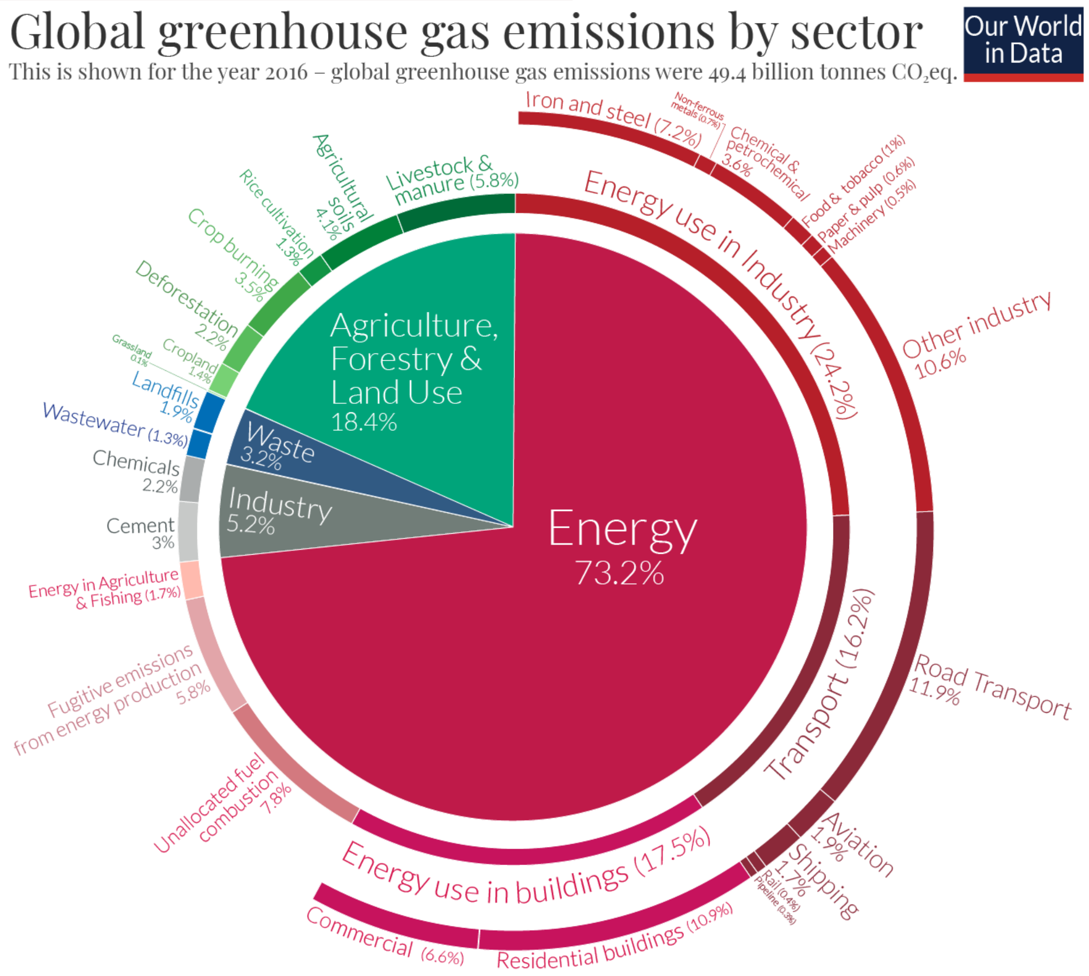
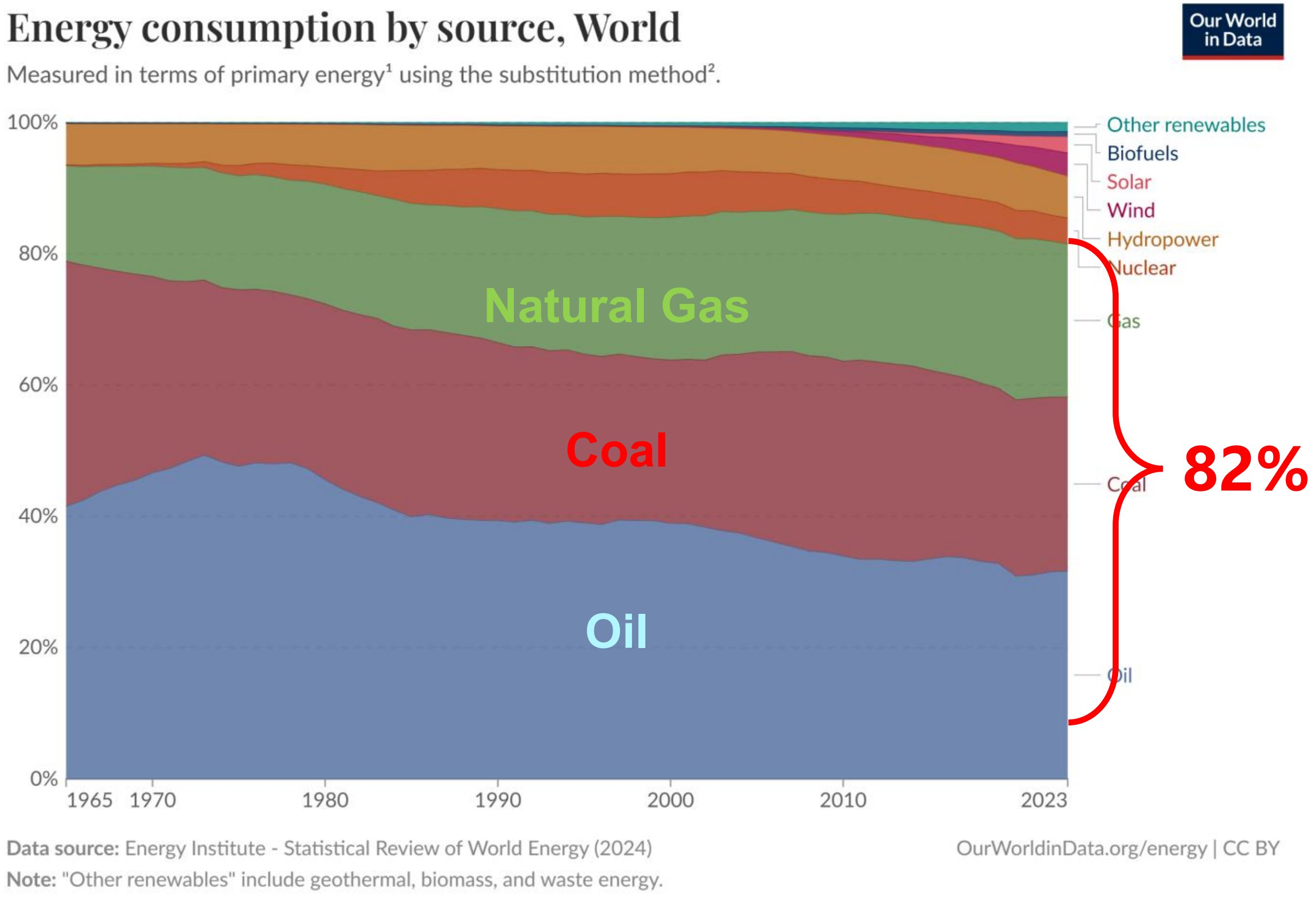
Why studying CO_2 capture?



Source : *https://ourworldindata.org/ghg-emissions-by-sector*



Source : *https://ourworldindata.org/grapher/energy-consumption-by-source-and-country*

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Why studying CO_2 capture?

① **AVOID**

Reducing global demand

② **SUBSTITUTE**

Replace fossil fuels with low-carbon energies

③ **UPGRADE**

CCUS

HECO2 – Saturn Project

- Funded by EU through Wallonia Region
  - Towards decarbonising Walloon heavy industry
    - Lime, Steel, Glass & Chemical sectors (Process-inherent CO_2 emissions)

- Goals of the project
  - Characterization of CO_2 emissions from industrial partners (AGC, APERAM, CARMEUSE & PRAYON)
  - Analysis and characterization of various CO_2 capture technologies
  - Modelling of different capture technologies (including LCA development)
  - Construction of a mobile cryogenic CO_2 capture unit
    - To be tested on the different industrial sites
  - Tests on a fixed CO_2 capture unit at CRM
    - Absorption-regeneration process using aqueous amine liquid solvent

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HECO2 – Saturn Project

Analysis and characterization of various CO_2 capture technologies

- Technology suppliers from around the world (47 listed)
  - Different technologies represented with hybrid ones

- Collaboration with UMons for this non-exhaustive list
- Handle information received from suppliers
  - Literature review
  - Modelling if needed

30 pages report including technologies description and comparison

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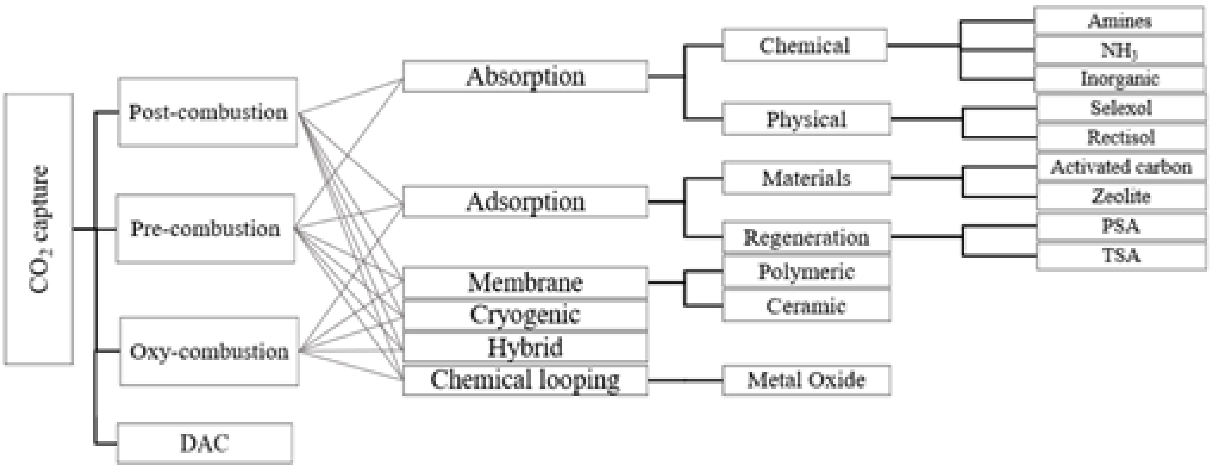
HECO2 – Saturn Project

Analysis and characterization of various CO_2 capture technologies

Increasing knowledge for DST operations

- **D**ecision **S**upport **T**ool for industrials to match their needs with the optimal CO_2 capture process
  - Which one will fit with my requirements? **Key Performance Indicators (KPIs)**
    - TRL
    - Purity
    - Impurity Tolerance
    - Installation footprints
    - CAPEX & OPEX
    - Safety Issues
    - Thermal and Electrical Energy Requirements
    - …



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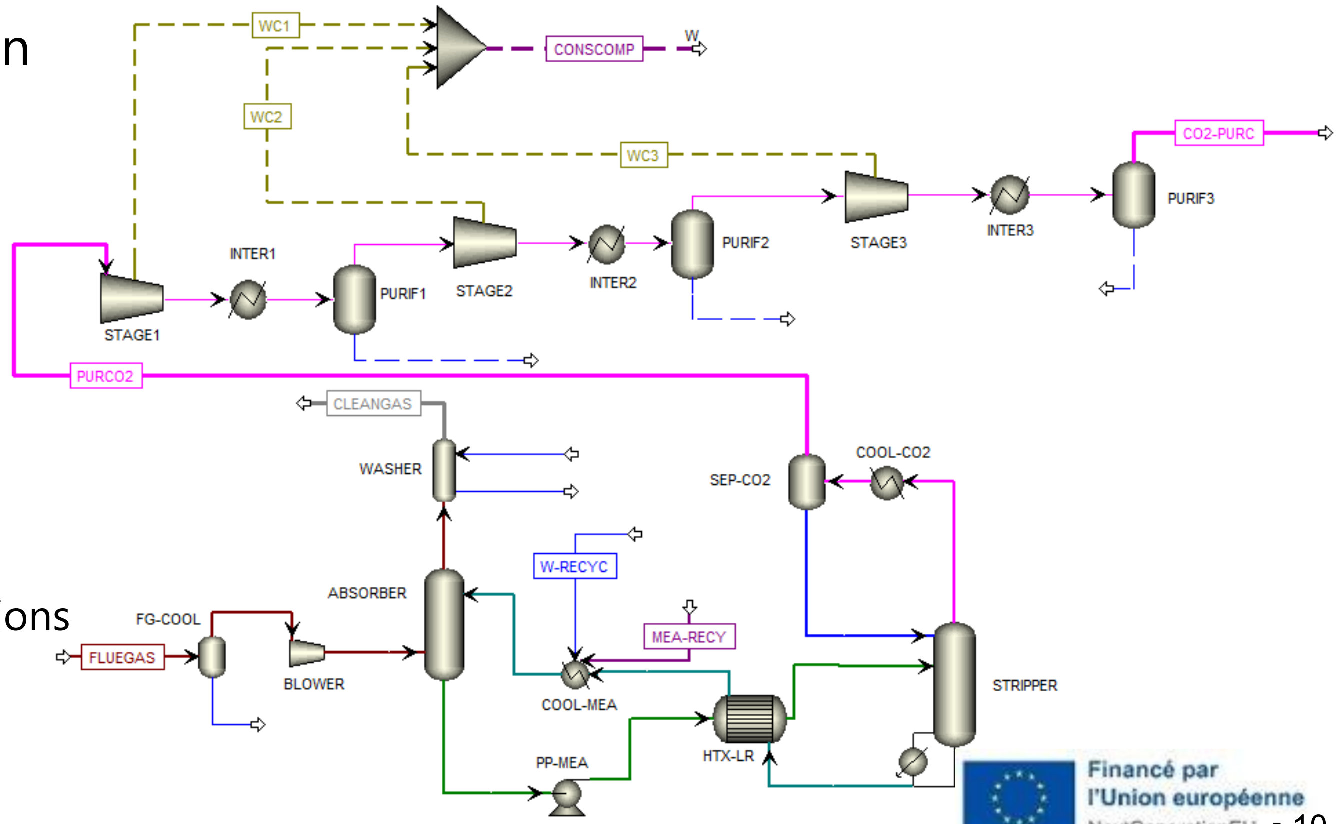
HECO2 – Saturn Project

Modelling of different capture technologies

Focus on MEA absorption-regeneration technology

- Benchmark solution for absorption
- High TRL
  - SaskPower's Boundary Dam Unit 3
    - 1 Mt/year
    - Saskatchewan (Canada)
- But nothing in Belgium
  - Adapted to Partners Flue Gas Conditions



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HECO2 – Saturn Project

Modelling of different capture technologies

- **Focus on MEA absorption-regeneration technology**
  - Consumption (3-4 GJ/t CO_2)
    - Waste Heat for some sectors → decreasing by 50 %
  - Cost: 150 – 160 €/t CO_2
    - Not including Transport
      - Neither transport specification (Fluxys, Northern Lights, …)

HECO2 – Saturn Project

Tests on a fixed CO_2 capture unit at CRM

- Modelling the entire pilot plant unit

Confidential

HECO2 – Saturn Project

Tests on a fixed CO_2 capture unit at CRM

Modelling the entire pilot plant unit

- Design of main equipment
- 15 base cases simulations
  - Flue gas composition
  - Amine flowrate
  - Work pressure
  - Amine solvent (MEA 30 wt.-%, AMP-PZ, ...)

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PhD Thesis

- Type of PhD
  - Experimental and Modelling
- Studied Processes
  - CO_2 capture process using absorption-regeneration technologies with amine solvent
- Application of the study
  - Process Industry in Wallonia
- Precise Topic
  - Acid gases and their impact on solvent degradation

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PhD Thesis

PEPs CHEMICAL ENGINEERING

"Experimental and Modeling Study of CO_2 Capture Processes by Absorption in Liquid Amine Solvents for Application in the Process Industry in Wallonia: Impact of SOx and NOx on Solvent Degradation"

Electrification CCUS HECO2 H_2

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PhD Thesis

PEPs CHEMICAL ENGINEERING

PhD Thesis of Prof. G. Léonard

- "Optimal design of a CO_2 capture unit with assessment of solvent degradation " (2013)
  - Oxidative and thermal degradation of MEA (monoethanolamine)
    - Ternary mixture (N_2 – O_2 – CO_2)
    - Degradation experiments on Test Bench (DTR)
    - Kinetic modelling of these degradation pathways

Electrification CCUS HECO2 H_2

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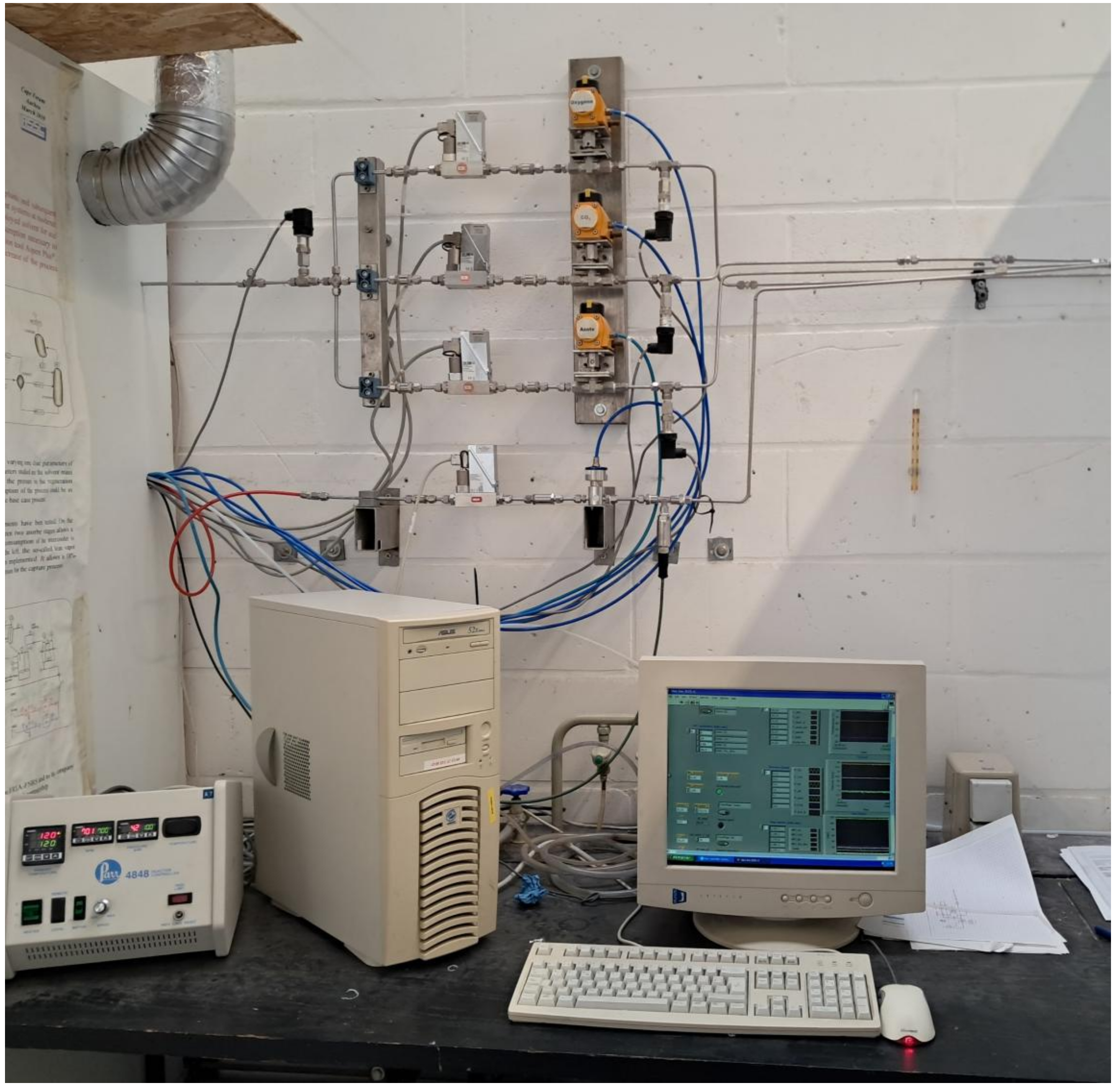
PhD Thesis

My PhD

- Extend the models to MEA degradation induced by SO_x & NO_x
  - Upgrade of the Degradation Test Rig
    - Quaternary Mixture (CO_2 – O_2 – N_2 – SO_x / NOx)
  - Analytical devices
    - HPLC-RID (MEA concentration)
    - GC-FID (Liquid degradation products)
    - IC (Anions → sulfate, formate, glycolate, acetate, … responsible for HSS)
    - FT-IR (NH_3 emission due to oxidative degradation)
    - ICP-MS (Metal cations due to corrosion)

PhD Thesis



PhD Thesis

My PhD

- Extend the models to MEA degradation induced by SO_x & NO_x
  - Reactions identification & Kinetic development
  - Inclusion to actual ASPEN models
    - Quantification of the impact on Energy Consumption
    - Quantification of MEA loss for CO_2 capture

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PhD Thesis

▶ SO_x influence

- Impact on the oxidative degradation (reactions between MEA and O_2)

$$SO_{2(g)} \longrightarrow SO_{2(aq)}$$

$$SO_{2(aq)} + H_2O_{(aq)} \longrightarrow H_2SO_{3(aq)}$$

$$H_2SO_3 \longrightarrow H^+_{(aq)} + HSO_3^-{}_{(aq)}$$

$$HSO_3^-{}_{(aq)} \longrightarrow H^+_{(aq)} + SO_3^{2-}{}_{(aq)}$$

$$2SO_3^{2-}{}_{(aq)} + O_{2(g)} \longrightarrow 2SO_4^{2-}{}_{(aq)}$$

$O_{2(g)}$ → Reduce O_2 availability for MEA degradation

$2SO_4^{2-}{}_{(aq)}$ → Acidification

- Production of Heat Stable Salts (HSS) with MEA^+
  - ▶ $SO_4^{2-} + 2\ MEA^+ \rightarrow HSS$

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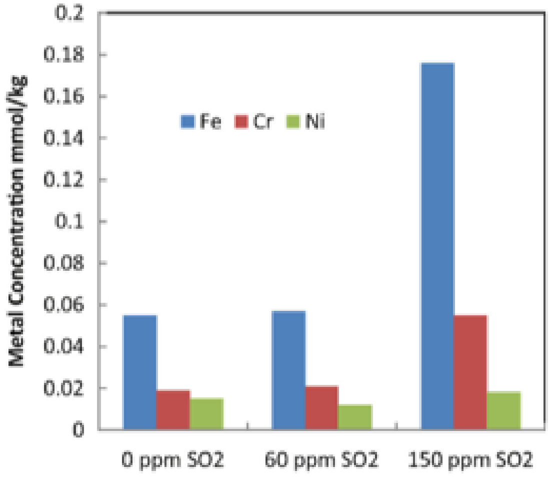
PhD Thesis

▶ SO_x influence

- Impact on the corrosion
  - Metal cations released into solution
    - Catalytic effect
      - Increasing products from oxidative degradation mechanisms



C. Sun, S. Wang, S. Zhou, and C. Chen, 'SO_2 effect on monoethanolamine oxidative degradation in CO_2 capture process', International Journal of Greenhouse Gas Control, vol. 23, pp. 98–104, Apr. 2014, Doi: 10.1016/j.ijggc.2014.02.010.

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PhD Thesis

Modelling part

- Modification of previous kinetics and inclusions of new ones

Rxn No.	Reaction type	Stoichiometry
1	EQUIL	MEAH+ + H2O <--> MEA + H3O+
2	EQUIL	2 H2O <--> H3O+ + OH-
3	EQUIL	HCO3- + H2O <--> CO3-2 + H3O+
4	KINETIC	OH- + CO2 --> HCO3-
5	KINETIC	HCO3- --> OH- + CO2
6	KINETIC	MEA + CO2 + H2O --> MEACOO- + H3O+
7	KINETIC	MEACOO- + H3O+ --> MEA + CO2 + H2O
8	KINETIC	MEA + 1,3 O2 --> 0,6 H3N + 0,1 HEI + 0,1 HEPO + 0,1 HCOOH + 0,8 CO2 + 1,5 H2O
9	KINETIC	2 MEA --> HEEDA + H2O
10	KINETIC	MEA + HEEDA --> TRIMEA + H2O
11	KINETIC	HEEDA + CO2 --> HEIA + H2O
12	KINETIC	TRIMEA + CO2 --> AEHEIA + H2O
13	KINETIC	2 MEA + CO2 --> BHEU + H2O
14	KINETIC	2 MEA + 0.5 O2 + SO2 + H2O --> 2 MEAH+ + SO4-2

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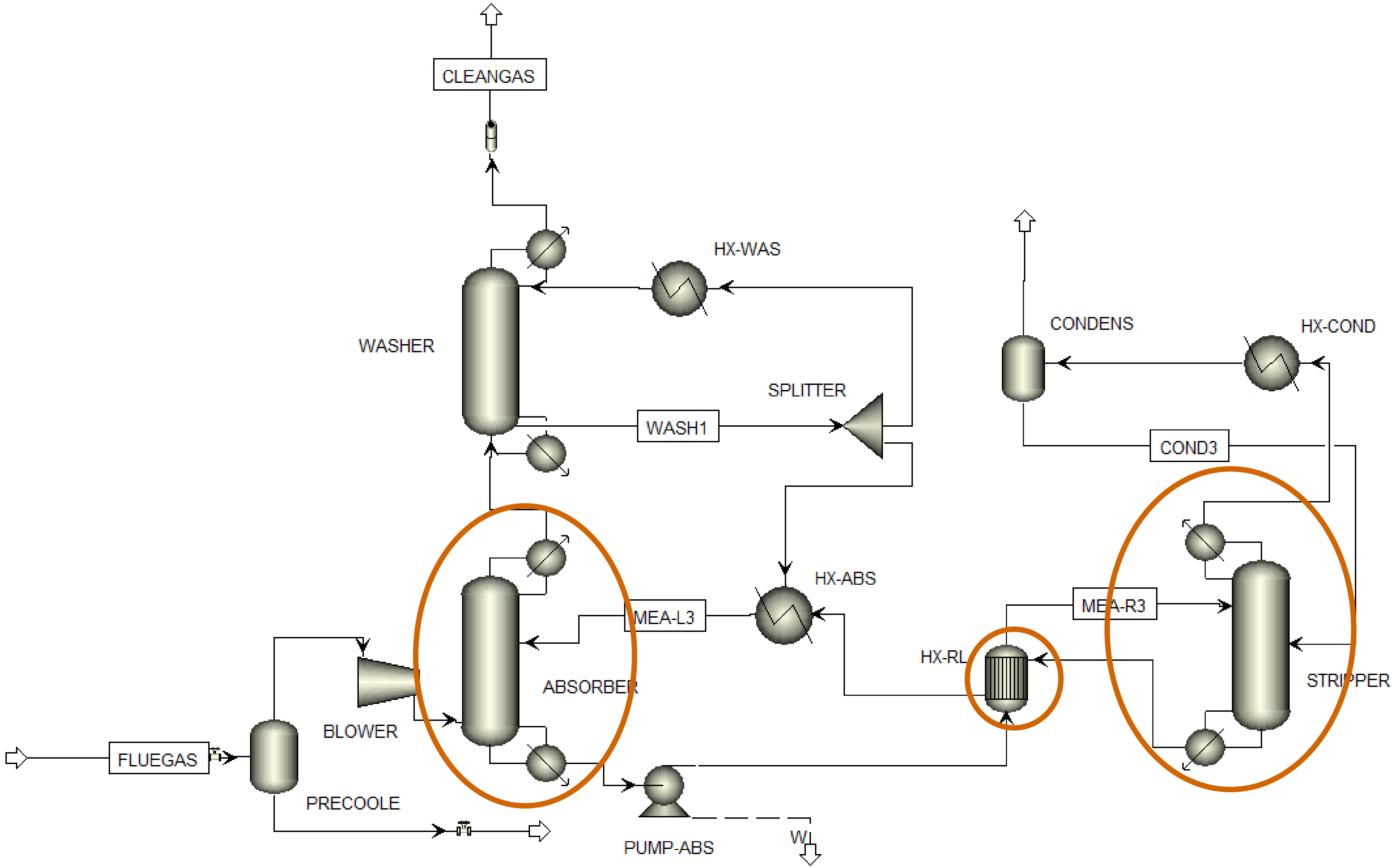
CLEANGAS
HX-WAS
WASHER
SPLITTER
WASH1
CONDENS
HX-COND
COND3
HX-ABS
MEA-L3
MEA-R3
HX-RL
ABSORBER
STRIPPER
BLOWER
FLUEGAS
PRECOOLE
PUMP-ABS
W

What's next?

- **Understanding deeply how SO_2 interact in the solution**
  - Varying experimental conditions in the DTR
    - $[O_2]$ & $[SO_2]$
    - Temperature
    - Pressure
  - Identify and quantify degradation products
    - Extract reaction mechanisms and kinetic parameters
  - Put it into simulation model

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General Conclusion

- CO_2 capture is a global topic with lots of interest
  - But there are still some missing parts
    - Degradation is still a hot topic for years
      - Proper solvent management will be key in addressing industrial reluctance toward implementation
- However, it is not the primary solution for fighting climate change
    - Keeping in mind the 3 principles
      - Avoid
      - Substitute
      - Upgrade

Thank you!

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